Slave Mode Expansion for Obtaining Ab Initio Interatomic Potentials and its Applications

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Abstract

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Having an interatomic potential overcomes limitations within DFT since it has a negligible cost in computing material properties while DFT is severely restricted by its computational cost when carrying out such tasks. In this thesis, we propose a new approach for creating an interatomic potential based on the Taylor series expansion of the crystal energy as a function of its nuclear displacements. We enlarge the dimensionality of the existing displacement space and form new variables (ie. slave modes) which transform like irreducible representations of the point group and satisfy homogeneity of free space. Standard group theoretical techniques can then be applied to deduce the non-zero expansion coefficients *a priori*. At a given order, the translation group can be used to contract the products and eliminate terms which are not linearly independent, resulting in a final set of slave mode products. By the end of the day, one ends up with an expansion that satisfies lattice symmetry and its number of coefficients is much smaller than that of a common Taylor series expansion. While the expansion coefficients can be computed in a variety of ways, we demonstrate that finite difference is effective up to fifth order. On the other hand, we demonstrate the power of the method in the strongly anharmonic systems PbTe and graphene. All anharmonic

terms within an octahedron are computed up to fourth order for PbTe, while those within a hexagon are computed up to fourth order and dimer terms are computed at fifth order for graphene. In addition, for PbTe, a proper unitary transformation of its potential demonstrates that the vast majority of the anharmonicity can be attributed to just two terms, indicating that a minimal model of phonon interactions is achievable. The ability to straightforwardly generate polynomial potentials will allow precise simulations at length and time scales which were previously unrealizable.

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Chapter 1

Introduction

In this thesis, we focus on two main topics: the introduction of a new approach that creates an interatomic polynomial potential for high-symmetry materials, and the assessment of the interatomic potentials created in the way that they predict materials' dynamic properties under strain. We would also shed light on their application in finite-temperature phonon spectrum. We shall begin with some general remarks on the fundamental limitations within DFT and how interatomic potentials overcome them. We will then briefly review a few existing methods that create interatomic potentials. Thereafter we would discuss some research areas where interatomic potentials surpass DFT in efficiency and accuracy – phonon instability and finite-temperature phonon spectrum.

1.1 Overcoming Limitations within DFT

Density functional theory (DFT)David Sholl (2009), within the framework of Born-Oppenheimer approximationBorn and Huang (1998), can accurately predict forces and stresses of many classes of materials and could therefore be used to compute both quantum and classical dynamics of the nuclei, including the harmonic vibrational properties of the crystals. However, the scaling of DFT severely restricts the applicability of such tasks to very short timescales and small unit cells and thus leads to some of its fundamental limitations in studying material properties. For example, since very large unit cells along with many time steps are needed to compute the anharmonic vibrational properties of the crystals at finite temperature even at the level of classical mechanics (also known as ab initio molecular dynamics), this in most cases renders DFT too expensive to compute them; and this is evidenced by the sparse number of such publications in the literature.

Generically, there are a number of different approaches to overcoming these fundamental limitations that exchange accuracy for efficiency. One of them uses an empirical interatomic potential in place of DFT. This is acceptable if an accurate empirical potential exists, but this is not always the case. In essence, they do not usually contain enough of the right physics or might be limited by the accuracy of the parametrization to describe the problem at hand, and correspondingly, their transferability to other environments could be poorAndreoni and Pastore (1990). There are also semi-empirical electronic structure approachesPapaconstantopoulos and Mehl (2003), and linear scaling DFTBowler and Miyazaki (2012); Vandevondele *et al.* (2012).

On the other hand, expanding the DFT energies as a function of the atomic displacements so that to form an interatomic potential provides an alternative solution to the dynamics of the nuclei, which in some cases is more accurate and efficient. For example, since the interatomic potential retains all the accuracy of DFT to a certain range and order while having a relatively negligible cost, it could be applied in molecular dynamics simulation so that the anharmonic vibrational properties of crystals at finite temperature could be studied accurately and efficientlyRavelo *et al.* (2013).

In this thesis, we will be introducing a new approach for interatomic potential construction that exceeds previous ones.

1.2 Methods to Achieve an Interatomic Potential

In general, the interatomic potential could be written down as a function of the atomic displacements based on the Born-Oppenheimer approximationLeSar (2013); Born and Huang (1998). It is shown as follows –

$$V = V(u_i, u_j, ..., u_k), \tag{1.1}$$

where indices i, j and k label both the atom and the cartesian coordinate. Because the atomic displacements could be further decomposed into subcomponents, e.g. uniform strain and sublattice shift and etc., the interatomic potential could actually have a lot of functional forms.

There are plenty of methods that could be used to achieve an interatomic potential and some of them would be presented in this section.

1.2.1 Earlier Works

Since the harmonic part of the interatomic potential could be computed using traditional approaches for computing phonons from first-principles, such as density functional perturbation theoryBaroni *et al.* (2001) or finite displacement supercell approachesAlfe (2009); Kunc and Martin (1982), most of the work is done to achieve its anharmonic part. Some of them were executed by Vanderbilt *et al.* in the context of SiVanderbilt *et al.* (1989) and by Rabe and Vanderbilt *et al.* in the context of ferroelectric materialsKingsmith and Vanderbilt (1994); Zhong *et al.* (1994, 1995). These approaches were quite successful, correctly capturing the proper ordering of different phases as a function of temperature and even providing quantitatively accurate transition temperatures.

Fundamentally, the earlier work of KeatingKeating (1966a,b) inspired a lot of them. In Keating's work, the elastic strain energy of a crystal is expanded in terms of a set of special variables so that the energy is invariant under an arbitrary displacement of the lattice. This set of variables are

$$\lambda_{klmn} = (\mathbf{x}_{kl} \cdot \mathbf{x}_{mn} - \mathbf{X}_{kl} \cdot \mathbf{X}_{mn})/2a, \tag{1.2}$$

where a is the lattice constant, $\mathbf{X}_{kl}$ is $\mathbf{X}_k - \mathbf{X}_l$, and $\mathbf{X}_k$ is the position vector of the kth nucleus in the undeformed crystal; they could also be chosen as

$$\lambda_{mn}(l) = (\mathbf{x}_m(l) \cdot \mathbf{x}_n(l) - \mathbf{X}_m(l) \cdot \mathbf{X}_n(l))/2a, \tag{1.3}$$

where l indexes the unit cells in the bulk and m,n indexes atoms within a unit cell and therefore sublattices – it is symmetric in (m, n). Thus, under small strains, the energy would be

$$E = \sum_{klmnpqrs} \frac{1}{2} B^{pqrs}_{klmn} \lambda_{klmn} \lambda_{pqrs}, \tag{1.4}$$

or

$$E = \frac{1}{2} \sum_{l,l'} \sum_{m,n,m',n'=1}^{4} B_{m'n'mn}(l - l') \lambda_{m'n'}(l') \lambda_{mn}(l), \tag{1.5}$$

where $\{B_{mnm'n'}(l-l')\}$ is invariant under the operations of the lattice vector translation group.

Because atomic displacements could be further written down as a uniform strain ϵ followed by a sublattice shift u_m(or internal strain indeed)–

$$\mathbf{x}_m(l) = (1 + \epsilon)\mathbf{X}_m(l) - u_m, \tag{1.6}$$

where l indexes the unit cells in the bulk and m indexes sublattices as in Eq. 1.3, the λ variables are actually functions of the macroscopic uniform strain variables $\eta = \epsilon + \frac{1}{2}\epsilon^2$ and internal strains. To be specific, $\lambda_{mn}(l)$ is equal to $\frac{1}{a_0}\sum_{a,b}\eta_{a,b}(l)X_m^a X_n^b$ in primitive structures and is a function of both uniform strain and internal strains in nonprimitive crystals. Though these internal strain variables do not exist in Keating's model since elastic strain energy only is studied, it inspires Vanderbilt's work on Si Vanderbilt *et al.* (1989).

In Vanderbilt's work, the energy of the Si crystal is therefore Taylor expanded in macroscopic uniform strains("acoustic" branch) and internal strains("optical" branch), retaining all terms up to combined fourth order. The total energy per two-atom unit cell could then be written in terms of the nine variables as follows –

$$\begin{aligned} E &= E(\eta_1, \eta_2, \eta_3, \eta_4, \eta_5, \eta_6, u_x, u_y, u_z) \\ &= E^{(0)} + E^{(2)} + E^{(3)} + E^{(4)} + ... \\ &= E^{(0)} + (E_{AA} + E_{AO} + E_{OO}) + (E_{AAA} + E_{AAO} + E_{AOO} \\ &+ E_{OOO}) + (E_{AAAA} + E_{AAAO} + E_{AAOO} + E_{AOOO} + E_{OOOO}), \end{aligned} \tag{1.7}$$

where Voigt notation is used – $\eta_1 = \eta_{xx}, \eta_4 = 2\eta_{yz}$, etc, and where A stands for "acoustic" branch and O stands for "optical" branch. For example, for crystals with cubic symmetry at harmonic order, one has

$$\begin{aligned} E_{AA} &= \frac{1}{2}B_{11}(\eta_1^2 + \eta_2^2 + \eta_3^2) + B_{12}(\eta_1\eta_2 + \eta_1\eta_3 \\ &\quad + \eta_2\eta_3) + \frac{1}{2}B_{44}(\eta_4^2 + \eta_5^2 + \eta_6^2), \\ E_{AO} &= B_{4x}(\eta_4 u_x + \eta_5 u_y + \eta_6 u_z), \\ E_{OO} &= \frac{1}{2}B_{xx}(u_x^2 + u_y^2 + u_z^2), \end{aligned} \tag{1.8}$$

where B_{11}, B_{12} and B_{44} are related by factors of the cell volume to the elastic constants of the crystal.

Thereafter, Vanderbilt incorporated a similar idea in the ferroelectric materials, as coupling to strain becomes critical in themKing-Smith and Vanderbilt (1994). An expansion similar to that of PytthePytte (1972) is applied to encode the properties of various perovskites. The energy per unit cell could be written as

$$E = E^0 + E^{disp}(\{v_\alpha^\tau\}) + E^{elas}(\{\eta_i\}) + E^{int}(\{\eta_i\}, \{v_\alpha^\tau\}), \tag{1.9}$$

where E^0 is the energy of the perfect perovskite structure. $E^{disp}(\{v_\alpha^\tau\})$ and $E^{elas}(\{\eta_i\})$

give a description of the energy to all orders at zero strain and zero displacement respectively. In crystals with cubic symmetry the strain energy is given, correct to second order in the strains, by

$$E^{elas}(\{\eta_i\}) = \frac{1}{2}B_{11}(\eta_1^2+\eta_2^2+\eta_3^2) + B_{12}(\eta_1\eta_2+\eta_1\eta_3 + \eta_2\eta_3) + \frac{1}{2}B_{44}(\eta_4^2+\eta_5^2+\eta_6^2), \tag{1.10}$$

the same as E_{AA} in Eqn. 1.8 given above.

Lattice Wannier Functions introduced by Rabe et al Iniguez *et al.* (2000) give rise to a new approach to achieving interatomic potential. They are actually symmetrized and localized basis of the atomic displacement modes within the lattice and could be achieved via a Fourier Transform of the normal modes which define the band subspace. They are symmetrized so that the number of expansion parameters needed are minimized; and they are localized therefore the intersite interactions are minimized.

There are potentials created using similar localized modes Zhong *et al.* (1994, 1995) and the following is an example–

$$E^{tot} = E^{self}(\{u\}) + E^{dpl}(\{u\}) + E^{short}(\{u\}) + E^{elas}(\{\eta_l\}) + E^{int}(\{u\},\{\eta_l\}), \tag{1.11}$$

in which

$$E^{self}(\{u\}) = \sum_i(\kappa_2 u_i^2 + \alpha u_i^4 + \gamma(u_{ix}^2u_{iy}^2 + u_{iy}^2u_{ix}^2 + u_{iz}^2u_{ix}^2)), \tag{1.12}$$

$$E^{dpl}(\{u\}) = \sum_{ij,\alpha\beta} Q_{ij,\alpha\beta}u_{i,\alpha}u_{j,\beta}, \tag{1.13}$$

with $Q_{ij,\alpha\beta} = \frac{2Z^{*2}}{\epsilon_\infty}[\frac{\pi}{\Omega_c}\sum_{G\neq 0}\frac{1}{|G|^2}exp(-\frac{|G|^2}{4\lambda^2})cos(G\cdot R_{ij})G_\alpha G_\beta - \frac{\lambda^3}{3\sqrt{\pi}}\delta_{\alpha\beta}\delta_{ij}]$ for perovskites where G is inverse lattice vector,

$$E^{short}(\{u\}) = \frac{1}{2}\sum_{i\neq j}\sum_{\alpha\beta} J_{ij,\alpha\beta}u_{i\alpha}u_{j\beta}, \tag{1.14}$$

$$E^{elas}(\{\eta_l\}) = E_I^{elas}(\{\eta_{I,l}\}) + E_H^{elas}(\{\eta_{H,l}\}), \tag{1.15}$$

(E_H^{elas}, the homogeneous elastic energy, has the same form with 1.10 in crystals with cubic symmetry; and E_I^{elas}, the inhomogeneous elastic energy, has more complicated forms concerning bond bending, bond correction and bond stretching etc. within the

lattice.) and

$$E^{int}(\{u\},\{\eta_l\}) = \frac{1}{2}\sum_i \sum_{l\alpha\beta} B_{l\alpha\beta}\eta_l(R_i)u_\alpha(R_i)u_\beta(R_i), \tag{1.16}$$

where u are the amplitudes of the localized modes and $\eta_l(R_i) = \eta_{H,l}(R_i) + \eta_{I,l}(R_i)$ – subscript I stands for inhomogeneous and subscript H stands for homogeneous.

1.2.2 Modern Works

With the continued explosion of computational resources, more recent works have revisited this problem. Esfarjani and Stokes considered the generic Taylor series expansion and all the symmetry constraints that the expansion must satisfyEsfarjani and Stokes (2008a). The following is the typical Taylar series expansion they used –

$$V = V_H(\sum_{ij}\Phi_{ij}u_iu_j) + \sum_{ijk}\Psi_{ijk}u_iu_ju_k + \sum_{ijkl}\chi_{ijkl}u_iu_ju_ku_l + ..., \tag{1.17}$$

where V_H is the harmonic contribution – Φ denotes harmonic force constants; Ψ and χ denote the third and fourth order force constants, respectively; u is the atomic displacement, while indices i, j, k and l label both the atom and the cartesian coordinate.

On the other hand, they used a lot of complex symmetry constraints that could be hard to implement. For example, to ensure the invariance of the energy under an arbitrary translation of the system, the following constraints are needed –

$$0 = \sum_\tau \Pi^\alpha_{0\tau}, \forall(\alpha)(\text{total force on unit cell=0}), \tag{1.18}$$

$$0 = \sum_{R_1,\tau_1} \Phi^{\alpha\beta}_{0\tau,R_1\tau_1}\forall(\alpha\beta,\tau), \tag{1.19}$$

$$0 = \sum_{R_2,\tau_2} \Psi^{\alpha\beta\gamma}_{0\tau,R_1\tau_1,R_2\tau_2}\forall(\alpha\beta\gamma,R_1,\tau_1), \tag{1.20}$$

$$0 = \sum_{R_3,\tau_3} \chi^{\alpha\beta\gamma\delta}_{0\tau,R_1\tau_1,R_2\tau_2,R_3\tau_3}\forall(\alpha\beta\gamma\delta,R_1R_2,\tau_1\tau_2), \tag{1.21}$$

where α, β, γ and δ could be x, y or z, R_i indexes unit cell (0 stands for the one at the origin) and τs index atoms within a unit cell; they are not straightforward to implement in fact.

They then generated a large data set from first-principles calculations and fit the expansion parameters to the data under the symmetry constraints. A number of materials and phenomena have been studied using this approach, including the thermal conductivity in SiEsfarjani *et al.* (2011), half-Heusler compoundsShiomi *et al.* (2011), and PbTeShiga *et al.* (2012).

Wojdel *et al.*Wojdel *et al.* (2013) employed a different approach, expanding in displacement differences between pairs of nuclei, similar in spirit to early model calculationsKeating (1966a,b), and they included point symmetry by projecting displacement difference polynomials onto the identity representation. Additionally, Wojdel *et al.* explicitly consider strain degrees of freedom and their coupling to local displacements, similar to earlier works in ferroelectric materials. In details, they started with the following energy expansion in displacement difference–

$$E = E_p(\{u_i\}) + E_s(\eta) + E_{sp}(\{u_i\}, \eta) + \text{long-range interactions}, \tag{1.22}$$

where

$$\begin{aligned} E_p(\{u_i\}) = &\frac{1}{2}\sum_{ijkh\alpha\beta} \widetilde{K}^{(2)}_{ij\alpha kh\beta}(u_{i\alpha} - u_{j\alpha})(u_{k\beta} - u_{h\beta}) \\ &+ \frac{1}{6}\sum_{ijkhrt\alpha\beta\gamma} \widetilde{K}^{(3)}_{ij\alpha kh\beta rt\gamma}(u_{i\alpha} - u_{j\alpha})(u_{k\beta} - u_{h\beta})(u_{r\gamma} - u_{t\gamma}) + ..., \end{aligned} \tag{1.23}$$

$$E_s(\eta) = \frac{N}{2}\sum_{ab} C^{(2)}_{ab}\eta_a\eta_b + \frac{N}{6}\sum_{abc} C^{(3)}_{abc}\eta_a\eta_b\eta_c + ..., \tag{1.24}$$

$$\begin{aligned} E_{sp}(\{u_i\}, \eta) = &\frac{1}{2}\sum_{a}\sum_{ij\alpha} \widetilde{\Lambda}^{(1,1)}_{aij\alpha}\eta_\alpha(u_{i,\alpha} - u_{j,\alpha}) \\ &+ \frac{1}{6}\sum_{a}\sum ijhk\alpha\beta\widetilde{\Lambda}^{(1,2)}_{aij\alpha kh\beta}\eta_a(u_{i\alpha} - u_{j\alpha})(u_{k\beta} - u_{h\beta}) \\ &+ \frac{1}{6}\sum_{ab}\sum_{ij\alpha} \widetilde{\Lambda}^{(2,1)}_{abij\alpha}\eta_a\eta_b(u_{i\alpha} - u_{j\alpha}) + ... \end{aligned} \tag{1.25}$$

They also group symmetry-related products together in the Taylor series, as their contribution to the energy is quantified by a common coupling coefficient and such a group is called a symmetry-adapted term(SAT). These SATs satisfy the point symmetry of the material spontaneously.

It is also worth mentioning recent machine learning approaches that have the potential to make a significant impact on constructing interatomic potentials. Behler

and Parrinello used a neural-network to parameterize the DFT energyBehler and Parrinello (2007), and they have achieved impressive results on NaEshet *et al.* (2010, 2012) and graphite/diamondKhaliullin *et al.* (2011). These results suggest that appropriate neural-networks have the potential to accurately describe structural phase transitions in a broad range of systems, though it is still unclear if they have sufficient resolution to accurately capture phonons and higher derivatives of the energy. Another approach in the context of machine learning is compressive sensing, which has been applied in the context of alloy theory to parameterize cluster expansionsNelson *et al.* (2013) and has also shown promise in the context of lattice dynamics.

1.2.3 Taylor Series Expansion

The Taylor series expansion of the energy as a function of the nuclear displacements, allowing for extremely high precision up to some order and within some range of neighbors, has been mentioned above. If one looks into the details of this approach, it is clear that it also has limitations. For example, it would not work if one studies large deformations of the lattice or if there is diffusion within the crystal lattice. However, as mentioned above, its computational cost is negligible relative to DFT and therefore allows length and timescales that could not even be considered within DFT. Therefore, in the regimes where it works, it overcomes the limitations of DFT and exceeds it. In addition, it has additional appeal in that its expansion coefficients are basic material properties. For example, the second order ones are force constants. What's more, understanding the anharmonic interactions across a broad range of materials will help understand a myriad of materials properties in terms of a low energy model. Our work in this thesis would be based on a Taylor series expansion while exceeding it. In essence, it has lattice symmetry, e.g. homogeneity of free space, group symmetry and lattice vector translational symmetry imposed *a priori*; therefore one not only needs not to use the complex symmetry constraints as in Stoke's workEsfarjani and Stokes (2008b) but also has less coefficients to be parameterized. Though the number of anharmonic terms rapidly increases with the order of the expansion, we will demonstrate in this thesis that there is reason to be optimistic that a minimal number of expansion coefficients can capture the bulk of the physics with an example in PbTe. While the Hubbard and Anderson models have guided us for many years in terms of understanding electronic phenomena in transition metal oxides and actinide based materialsKotliar *et al.* (2006), analogues are clearly needed in the context of the interacting phonon problem.

1.3 Areas where Interatomic Potentials Exceed DFT

There are various areas where interatomic potentials exceed DFT in efficiency and accuracy. For example, when phonon instability with respect to lattice strain is studied in DFT or DFPT, one needs to recompute phonon frequencies for different lattice structures. However, if one is given an interatomic potential, the new phonon frequencies associated with a different lattice structure could be conveniently obtained by renormalizing the harmonic terms using the anharmonic onesAi *et al.* (2014). What's more, while computing the finite-temperature phonon spectrum within the framework of DFT is expensive, using an interatomic potential could be much cheaperChen *et al.* (2014). These are our motivations to generate interatomic potentials.

1.3.1 Phonon Instability

Research done on phonon instabilities are getting more and more essential as they control the ideal strength of a defect-free crystal at 0K and is therefore influential on materials' mechanical properties – when a phonon mode goes soft or a related stress-strain curve bends down, the material could break or undergo some phase transitionA.Kelly (1987). For example, ideal strength is ultimately dictated by the elastic instability, known as phonon instability at Γ point. Aside from elastic instability, it could also be limited by a finite-wavevector phonon instability, or a soft mode, occurring at a lower stress than that of the elastic instability; and such phonon instabilities have been predicted to limit the ideal strength of bulk aluminumClatterbuck *et al.* (2003) and bulk siliconDubois *et al.* (2006). In this section, we would be giving some examples on phonon instabilities of graphene under different types of lattice strains – tensions along armchair direction and zigzag direction, or equibiaxial strain.

To study graphene's phonon instabilities under tensions along armchair direction and zigzag direction, Ju Li *et al.* compute the phonon dispersions and stress-strain curvesLiu *et al.* (2007). From phonon dispersion studies, they found that under both tensions, phonon instabilities occur near the center of the Brillouin zone. What's more, the phonon instability under armchair tension occurs at $\varepsilon_{xx} = 0.194$, $\sigma_{xx} = 110GPa$ and $\varepsilon_{yy} = -0.016$ and that under ziazag tension occurs at $\varepsilon_{yy} = 0.266$, $\sigma_{yy} = 121GPa$ and $\varepsilon_{xx} = -0.027$, respectively. These are clear in Fig. 1.1 and Fig. 1.2. On the other hand, the stress-strain curves computed using primitive cells of graphene in Fig. 1.3 yield the same results in predicting the strains where the phonon instabilities occur.

Then one would argue that stress-strain curve is cheap to achieve in DFT and that facilitates the research on ideal strength. Nevertheless, this is only true in case that one

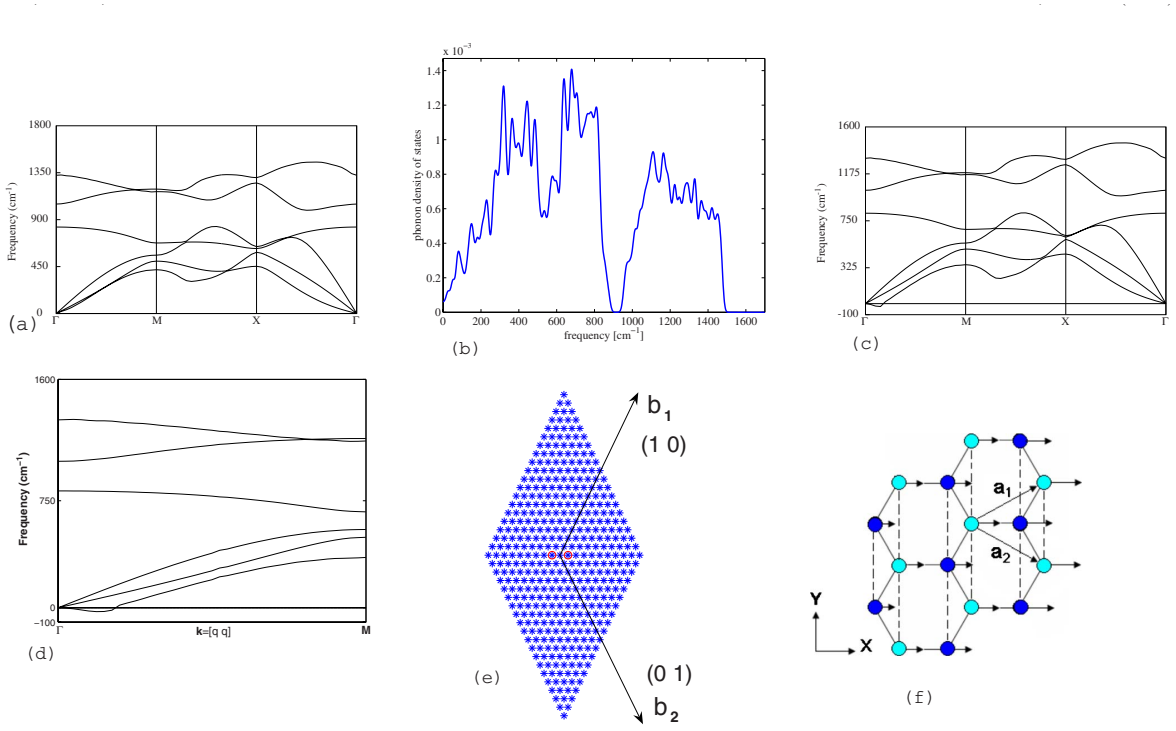

Figure 1.1: (a) Phonon dispersion and (b) density of states of graphene at $\varepsilon_{xx} = 0.18$. There is no soft mode yet. (c) Phonon dispersion at ε_{xx}=0.194, $\sigma_{xx} = 110$GPa. (d) Blow-up of the unstable branch along $\mathbf{k} = \mathrm{q}(b_1 + b_2) = \mathrm{k}e_x$. (e) Scan of the entire Brillouin zone at $\varepsilon_{xx} = 0.194$ to make sure that (d) is the first phonon instability. (f) The unstable eigenvector corresponding to the softmode at $\varepsilon_{xx} = 0.194$. (from paper Liu *et al.* (2007))

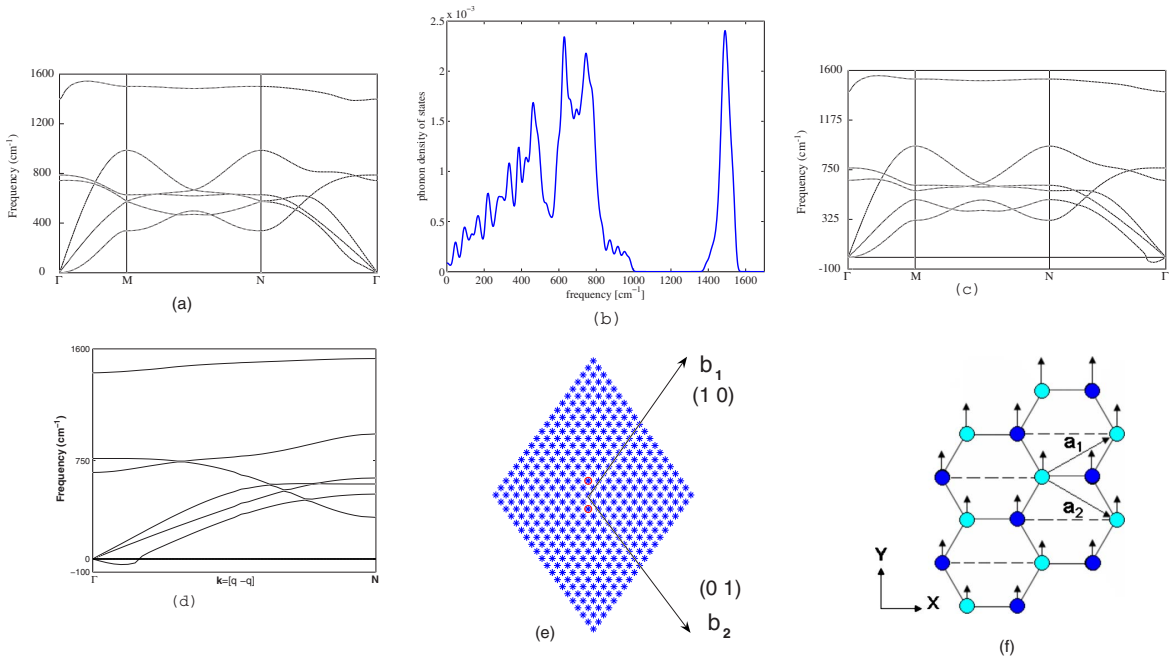

Figure 1.2: (a) Phonon dispersion and (b) density of states of graphene at ϵ_{yy} =0.24. There is no soft mode yet. (c) Phonon dispersion at $\epsilon_{yy} = 0.266$, $\sigma_{yy} = 121$ GPa. (d) Blow-up of the unstable branch along $\mathbf{k}$ = q(b_1 - b_2) = ke_y. (e) Scan of the entire Brillouin zone at $\epsilon_{yy} = 0.266$ to make sure (d) is the first phonon instability. (f) The unstable eigenvector corresponding to the soft mode at $\epsilon_{yy} = 0.266$. (from paper Liu *et al.* (2007))

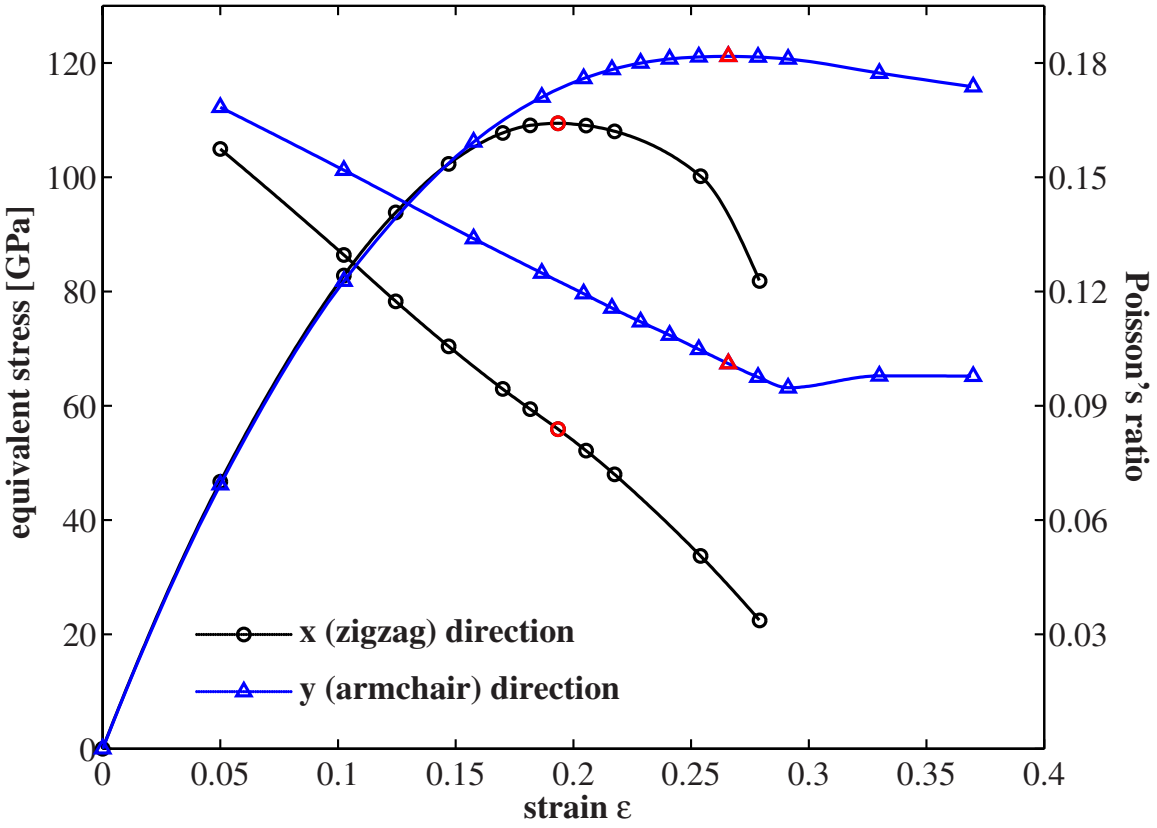

Figure 1.3: The curves connected to the origin are the equivalent tensile stress ($d_0 = 3.34\mathring{A}$) versus uniaxial strain in the x and y directions, respectively. The lines with initially negative slopes (scale labels to the right) are the finite-deformation Poisson's ratios as functions of the uniaxial strain in the x and y directions, respectively. The red circles and triangles indicate the condition where peak stress could be attained for zigzag and armchair nanotubes, respectively. (from paper Liu *et al.* (2007))

knows which phonon mode limits the ideal strength of the material being studied and the corresponding stress-strain curve could be computed using a relatively small unit cell. For example, in the above case, after knowing that the phonon instability occurs first near the center of the Brillouin zone, one just need to compute the stress-strain curve with a primitive cell.

However, there are materials whose ideal strengths are limited by finite-wavevector phonon modes. For example, the ideal strength of graphene is limited by the K-point phonon mode under equibiaxial strainMarianetti and Yevick (2010). In this case, one has to compute the strains predicted by K-cell, as shown in Eric Isaacs and C. A. Marianetti's workIsaacs and Marianetti (2014). The same is also true for some other two-dimensional materials they study and the comparisons between the stress-strain curves computed using primitive cells and K-cells are shown in Fig. 1.4. This means that the phonon dispersions still have to be computed for different structures before one could dig into more details via the stress-strain curve and an interatomic potential would exceed DFT in efficiency.

1.3.2 Finite Temperature Phonon Spectrum

If phonon instabilities dictate the ideal strength of materials under zero temperature, finite-temperature phonon spectra would help in figuring out the ideal strength and other mechanical properties of materials under finite temperature. However, the finite-temperature phonon spectrum could not be computed directly within the framework of DFT at present and one would need some other tools for assistance. For example, with molecular dynamics and DFT, the finite-temperature phonon spectrum could be computed for Li, which is shown in Fig. 1.5 Hellman *et al.* (2011). In addition, though the result agrees well with the experimental one, they used a 128-atom bcc supercell and a total of 44000 time steps, which is incredible in DFT. On the other hand, there are materials whose harmonic coupling decays slowly and a much larger supercell would be needed in the calculation. For example, an 8000-atom bcc supercell is used in the molecular dynamics study of PbTeChen *et al.* (2014). It means that DFT could be unnecessarily inconvenient and expensive when studying the finite-temperature phonon spectra of materials and therefore an interatomic potential for molecular dynamics simulation would be desired.

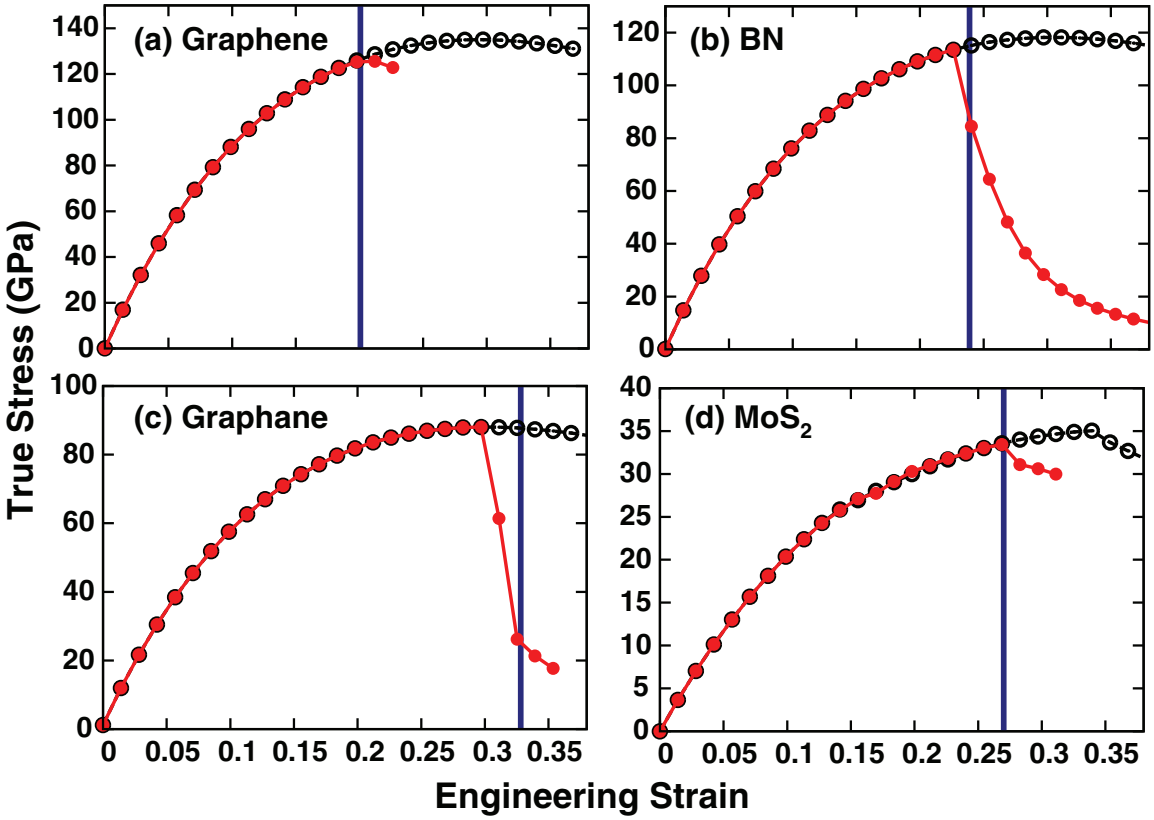

Figure 1.4: The stress σ vs. engineering strain ε for (a) graphene, (b) BN, (c) graphane, and (d) MoS2 under equibiaxial strain. Black lines and open circles are for the primitive unit cell; red lines and solid circles are for the K cell. The strain at which a phonon mode goes soft at the K point is indicated by a blue line. (from paper Isaacs and Marianetti (2014))

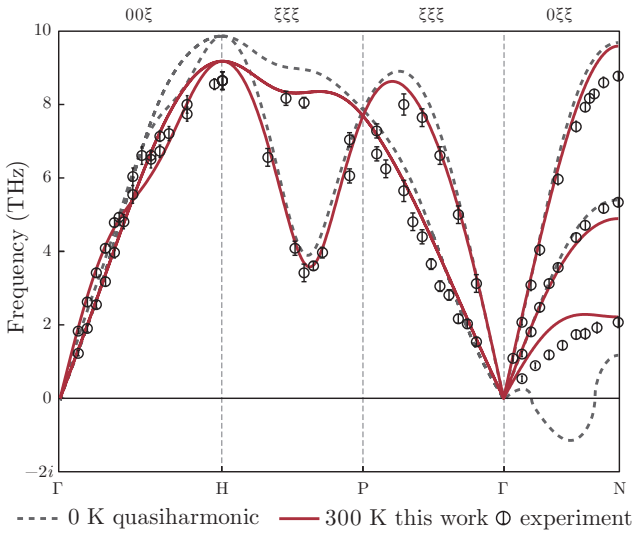

Figure 1.5: Phonon dispersion relations in bcc Li along high-symmetry directions. The symbols are experimental values (293K)Beg and Nielsen (1976), the solid lines correspond to calculations carried out at 300K using DFT and molecular dynamics, and the dashed black lines correspond to the 0K harmonic calculations. (from paper Hellman *et al.* (2011))

Chapter 2

Theory

As one could figure out from the Introduction, despite the great successes of the previous expansions, they have not yet become ubiquitous – perhaps because it is nontrivial to execute the parametrization. In this thesis we would introduce a new approach which combines many of the advantages of the different methods discussed above but has symmetries built in from the beginning and therefore less coefficients to be determined. It allows us to circumvent the difficulties of imposing necessary symmetries afterwards and fitting data across multiple orders, and provides a convenient notation to encode our parameters such that others may use them.

In this chapter, we are going to derive this new approach - slave mode expansion - for obtaining interatomic potentials for materials. We would start by writing down a Taylor series expansion for the interatomic potential, which could be upgraded to one in difference representation to impose the homogeneity of free space under translation. The improved expansion in a 1d chain sheds light on a slave mode expansion in this simple case. Thereafter a symmetrized monomial representation in which the majority of the symmetries could be imposed on the Taylor series step by step *apriori* is introduced and it gives rise to the slave mode expansion in general. Last but not least, the formal presentation of the slave mode expansion would be given.

2.1 A General Taylor Series Expansion and Difference Representation

The Born-Oppenheimer approximationBorn and Huang (1998) separates the nuclear degrees of freedom from those of the electrons in a many-body problem and renders it convenient to solve for crystal energies using an interatomic potential. The interatomic potential could actually be written down as a Taylor series in terms of atomic displacement products as followsEsfarjani and Stokes (2008a):

$$
\begin{aligned}
V = & \sum_{\alpha\beta\mathbf{R}_a\mathbf{R}_b} \Psi^{\alpha\beta}_{\mathbf{R}_a\mathbf{R}_b} u^{(\alpha)}_{\mathbf{R}_a} u^{(\beta)}_{\mathbf{R}_b} \\
& + \sum_{\substack{\alpha\beta\gamma \\ \mathbf{R}_a\mathbf{R}_b\mathbf{R}_c}} \Psi^{\alpha\beta\gamma}_{\mathbf{R}_a\mathbf{R}_b\mathbf{R}_c} u^{(\alpha)}_{\mathbf{R}_a} u^{(\beta)}_{\mathbf{R}_b} u^{(\gamma)}_{\mathbf{R}_c} \\
& + \sum_{\substack{\alpha\beta\gamma\delta \\ \mathbf{R}_a\mathbf{R}_b\mathbf{R}_c\mathbf{R}_d}} \Psi^{\alpha\beta\gamma\delta}_{\mathbf{R}_a\mathbf{R}_b\mathbf{R}_c\mathbf{R}_d} u^{(\alpha)}_{\mathbf{R}_a} u^{(\beta)}_{\mathbf{R}_b} u^{(\gamma)}_{\mathbf{R}_c} u^{(\delta)}_{\mathbf{R}_d} + \cdots
\end{aligned}
\tag{2.1}
$$

Where Ψ are the direct expansion coefficients, u are the atomic displacements, $\mathbf{R} = n_1\mathbf{v}_1 + n_2\mathbf{v}_2 + n_3\mathbf{v}_3$ (n_i are integers, $\mathbf{v}_i$ are unit cell vectors), $\alpha, \beta, \gamma, \delta$ label both the displacement direction (i.e. x, y, z) and the atom within the unit cell. As the order increases, the number of terms increases dramatically. Therefore, this expansion is only useful when interactions, especially high-order ones, decay quickly with distance so that most of the coefficients are small compared with dominant ones at that order and could be ignored. This is true in a lot of materials, and this is why the Taylor series expansion is useful in previous works.

However, one drawback of this general expansion is that it's not constrained by symmetry while there are a lot of them in a lattice. The first one is homogeneity of free space - if a crystal is translated or rotated, no energy change is allowed. What's more, there are also a lot of space group operations that the crystal energy should be invariant under. Moreover, if a cluster of atoms could be translated to another one by lattice vectors, the energies of atomic displacements within either of the clusters should be the same. Therefore, lots of constraints on the expansion coefficients are needed to enforce these symmetries so that the resulting potential is useful in real applicationsEsfarjani and Stokes (2008a). Even though, imposing the constraints by adding in some equations during the parametrization process leads to a lot of unpredictable trade-offs that might give rise to severe problems. For example, when the crystal is shifted with a very large movement, the Taylor series expansion might suffer or even wouldn't work because homogeneity of free space might have been sacrificed a little bit.

Nevertheless, these worrisome constraints will be dispensable if one could have the symmetries imposed *apriori*. For exmaple, if the atomic displacements in a Taylor series expansion are replaced by differences between them, no further constraints on the homogeneity of free space will be needed after the potential is formulated. We will call this new series an expansion in difference representation. In this approach, the number of degrees of freedom, as well as the number of coefficients in the expansion, is reduced. On the other hand, if one could have more symmetries imposed *apriori*, the

number of coefficients would be further reduced.

2.2 1-d Chain – Difference Representation Sketching a Slave Mode Expansion

The expansion in difference representation for the potential of a 1-d monoatomic chain sketches a slave mode expansion in this simple case when the couplings beyond nearest neighbor are ignored. With nearest neighbor coupling considered only, the expansion for the potential of this chain in difference representation would be a Taylor series in terms of different orders of $(x_i - x_{i-1})$ with i going from the first to last atom in the chain. One could also write down the terms in each of the 2-atom cluster $(atom_{i-1}, atom_i)$ and sum over the lattice. On the other hand, the 2-atom clusters have point group C_2, which contains the identity E and the mirror σCornwell (1997); Tinkham (1964) and the character table for this group has two possible irreducible representations, the symmetric and asymmetric irreducible representation denoted as A, or identity and stands for quantities that are invariant under arbitrary point symmetry operations, and B. It is not hard to realize that $(x_i - x_{i-1})$ is actually A and orders of it are still As according to point group theory. This not only indicates that the Taylor series in difference representation satisfies both the translational part of homogeneity of free space and point symmetry of C_2, but also inspires the thinking of expanding the potential directly using products of atomic displacement modes that transform like A at all orders. One might wonder whether the other mode B should be included in such an expansion or not since its higher order products could also transform like identities – the answer is a straightforward no because B mode as $(x_i + x_{i-1})$ does not satisfy the homogeneity of free space. Therefore, one could define such a series of identity representations constructed from the atomic displacement modes orthogonal to pure translations a slave mode expansion and the expansion in difference representation for 1d chain is exactly it.

2.3 Symmetrized Monomial Representation

Generally, the majority of symmetries discussed in Sec. 2.1 could be imposed on the expansion step by step *apriori*. In fact, one could build a local space with basis being

monomials of atomic displacements within an atomic cluster defined by a coupling range and successively reduce its dimensionality by imposing the various symmetries.

To realize this, the potential in equation 2.1 should be rewritten using the new basis as follows:

$$V = \sum_{\mathbf{R}_a n} \mathbf{\Psi}_n \xi^{(n)}_{\mathbf{R}_a} = \sum_{\mathbf{R}_a n} \mathbf{\Psi}_n \hat{\mathbf{\Gamma}}^{-1}_n \hat{\mathbf{\Gamma}}_n \xi^{(n)}_{\mathbf{R}_a} \tag{2.2}$$

where n labels the order of the polynomial, ξ is a vector with each entry being a monomial, R_α denotes which site the atomic cluster is on and $\mathbf{\Psi}$ is a vector of the direct expansion coefficients. The atomic displacements within an atomic cluster is collected by $\mathcal{S}$. If the coupling between displacements in the lattice is cut beyond a certain distance so that the length of $\mathcal{S}$, $|\mathcal{S}|$, equals to z at order n, then the dimensionality of ξ, as well as the number of distinct monomials for $\mathcal{S}$, at that order is going to be the k-multicombination and

$$\dim(\xi^{(n)}) = \left(\binom{z}{n}\right) = \binom{z+n-1}{n} = \frac{(z+n-1)!}{n!(z-1)!}. \tag{2.3}$$

This number increases dramatically with z and n and for this expansion to be useful, especially when order is high, the coupling should decay quickly so that one ends up with a small z.

Then it's straightforward that the expansion by construction satisfies lattice vector translational symmetry by taking up terms with the same structure from each $\mathbf{R}_a$. Therefore one only needs to impose the various other symmetries on the invertible linear transformation matrix $\hat{\mathbf{\Gamma}}_n$, which stands for rotations or dimensionality reductions of the monomial vectors without changing any physical observables. The change in the shape of Γs, i.e. the decrease in its number of rows when these symmetries are being built in, means that the number of paramters will be reduced. The homogeneity of free space with respect to rigid rotations would be ignored because it couples terms between different orders but it wouldn't be too problematic because symmetries with respect to discrete rotations, i.e. point symmetries, are imposed.

2.3.1 Point Symmetry

Intuitively, because of point group symmetry, a lot of the monomials at a specific order are equivalent to each other. It implies that one could reduce the dimensionality of local space by replacing them with their sum, or replacing a bunch of equivalent

vector basis by their sum as a new basis without changing the potential.

Theoretically, in point group theory, the representation formed by the monomials at a specific order, e.g. n, are reducible at most of the time and could be decomposed into irreducible ones including the identity, the one invariant under any point symmetry again, according to the standard techniques of group theoryCornwell (1997); Tinkham (1964). In particular, the point group could be represented by a set of symmetry operation matrices that are square and of dimension $\dim(\xi^{(n)})$ by $\dim(\xi^{(n)})$ in the space spanned by the $\dim(\xi^{(n)})$ basis vectors for nth order monomials and the irreducible representations would then be vectors of monomials that block diagonalize them and could be further identified via the character number. The identities are those with all character numbers being 1 and would form a new complete basis for potential expansion after linearly independent ones are removed since only the identity representations have non-zero expansion coefficients in a potential. They could actually be achieved directly by applying the projection operator on each of the $\dim(\xi^{(n)})$ basis vectors and collect the linearly independent vectors after projection.

Finally, the square matrix $\hat{\mathbf{\Gamma}}$ is reduced to a rectangular matrix $\hat{\mathbf{\Gamma}}'$ with less number of rows than columns given that representations that are not the identities are removed, and each row of the rectangular matrix actually correspond to a given identity representation of monomials.

$$V = \sum_{\mathbf{R}_a n} \mathbf{\Psi}_n \hat{\mathbf{\Gamma}}'^{-1}_n \hat{\mathbf{\Gamma}}'_n \xi^{(n)}_{\mathbf{R}_a} = \sum_{\mathbf{R}_a n} \mathbf{\Psi}'_n \hat{\mathbf{\Gamma}}'_n \xi^{(n)}_{\mathbf{R}_a} \tag{2.4}$$

It is implicit in the above that $\hat{\mathbf{\Gamma}}'^{-1}_n$ is the left-inverse of the rectangular matrix $\hat{\mathbf{\Gamma}}'_n$.

2.3.2 Homogeneity of Free Space

Enforcing homogeneity of free space would lead to further row removals of matrix $\hat{\mathbf{\Gamma}}'_n$ or linear combinations of its different rows, so that the energy and its derivatives would remain unchanged if the entire crystal is shifted. In details, one needs to consider the shift of the crystal in x, y, and z directions by arbitrary constants, in addition to all permutations of combined shifts; these shifts would then result in a set of monomial vectors $\{\xi^{(n)}_1, \xi^{(n)}_2, \cdots\}$ and enforcing the homogeneity of free space would form constraints on them. Additionally, the derivatives for each inequivalent atomic displacement in the unit cell should be considered, and these must also remain invariant with respect to an arbitrary shift. For a given derivative, this must be true independently for contributions from each order. For example, the n-th order contribution to

the first derivative is given as follows:

$$\begin{aligned}\frac{\partial V^{(n)}}{\partial u_0^{(\alpha)}} &= \mathbf{\Psi'}_n \hat{\mathbf{\Gamma}}'_n \sum_{\mathbf{R}_a} \frac{\partial}{\partial u_0^{(\alpha)}} \xi^{(n)}_{\mathbf{R}_a} \\ &= \mathbf{\Psi'}_n \hat{\mathbf{\Gamma}}'_n \eta^{(n,1)}_\alpha \end{aligned} \tag{2.5}$$

The vector $\eta^{(n,1)}$ must then be shifted by arbitrary amounts in the x, y, z directions and all permutations thereof, and enforcing the homogeneity of free space would end up with constraints on them. This procedure is then repeated for all higher order derivatives up to $n-1$. Finally, we will have formed a set of vectors $\mathcal{L}_n = \{\xi^{(n)}_1, \xi^{(n)}_2, \cdots, \eta^{(n,1)}_{\alpha,1}, \eta^{(n,1)}_{\alpha,2}, \dots\}$. One then proceeds by finding the number of linearly independent vectors in $\mathcal{L}_n$, denoted as $N_{\mathcal{L}_n}$, and then constructing $N_{\mathcal{L}_n}$ vectors from $\mathcal{L}_n$ which span this space. Enforcing the homogeneity of free space would thus result in $N_{\mathcal{L}_n}$ unique constraints at order n, and this will remove up to $N_{\mathcal{L}_n}$ rows from $\hat{\mathbf{\Gamma}}'_n$, guaranteeing homogeneity of free space. The resulting potential can then be written as follows:

$$V = \sum_{\mathbf{R}_a n} \mathbf{\Psi''}_n \hat{\mathbf{\Gamma}}''_n \xi^{(n)}_{\mathbf{R}_a} \tag{2.6}$$

2.3.3 Lattice Translations

Because at most of the time the clusters overlap with each other in the lattice and one sums up clusters on each site so that the potential satisfies the translation group, terms that are different viewed inside a cluster may not be when viewed at the level of the lattice – indicating there might be further row removals in $\hat{\mathbf{\Gamma}}''$.

This could be realized after the following analysis and procedures. For atomic displacements within an atomic cluster on site $\mathbf{R}_0$ that are contained by $\mathcal{S}_0$, they not only contribute to monomials in vector $\xi^{(n)}_{\mathbf{R}_0}$ for cluster on site $\mathbf{R}_0$ but also contribute to those in vectors for neighboring clusters. Mathematically, the following equation shows what it means,

$$\sum_{\mathbf{R}_a} \hat{\mathbf{\Gamma}}''_n \xi^{(n)}_{\mathbf{R}_a} \Big|_{u^{(\alpha)}_{\mathbf{R}_a} \notin \mathcal{S}_0 \to 0} = \hat{\mathcal{V}}_n \xi^{(n)}_{\mathbf{R}_0}. \tag{2.7}$$

If the rank of $\hat{\mathcal{V}}_n$ is less than the number of rows, there is linear dependency at the level of the lattice among the terms that are not within a cluster and the corresponding

rows could be removed. Finally its rank ends up to be equal to its number of rows and we end up with identities that are linearly independent basis for the potential. The same row contraction should be performed on $\hat{\mathbf{\Gamma}}''_n$, yielding the final potential:

$$V = \sum_{\mathbf{R}_a n} \mathbf{\Phi}_n \hat{\mathbf{\Gamma}}'''_n \xi^{(n)}_{\mathbf{R}_a} \tag{2.8}$$

where the symbol $\mathbf{\Psi}_n$ is now changed into $\mathbf{\Phi}_n$ in order to emphasize that a fully irreducible set of expansion coefficients have been achieved.

2.3.4 Illustration in 1-d Chain

The symmetrized monomial representation outlined above could be illustrated using a simple example of the monoatomic one-dimensional chain. As mentioned before, the point group of 1-d chain is C_2 and the character table for it has two possible irreducible representations, the symmetric and asymmetric irreducible representation denoted as A and B, respectively. We will assume that the range of the coupling is next-nearest neighbor, and therefore the atomic cluster on $\mathbf{R}_0$ contain atomic displacements $u_{\bar{1}}$, u_0 and u_1, and so that $\mathcal{S}_0 = \{u_{\bar{1}}, u_0, u_1\}$. At quadratic order, the monomial vector has $\left(\binom{3}{2}\right) = 6$ entries:

$$\hat{\xi}^{(2)}_0 = \begin{pmatrix} u^2_{\bar{1}} & u^2_0 & u^2_1 & u_{\bar{1}}u_0 & u_{\bar{1}}u_1 & u_0u_1 \end{pmatrix}^\intercal \tag{2.9}$$

Without symmetry, there would be one independent Ψ parameter for each monomial and Γ would be 6 by 6 square. However, when C_2 point symmetry is included, the standard techniques of group theory could be applied and there would be four irreducible representations left that transform as the identity representation:

$$\hat{\mathbf{\Gamma}}'_2 = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix} \tag{2.10}$$

The next step is to enforce homogeneity of free space, and therefore we construct the vector space $\mathcal{L}$. We will consider both the energy and the force (ie. only one type of

atom and one spatial dimension) under a uniform shift $\delta = 1$, resulting in two vectors:

$$\mathcal{L} = \left\{ \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 \end{pmatrix}^\intercal, \begin{pmatrix} 2 & 2 & 2 & 2 & 2 & 2 \end{pmatrix}^\intercal \right\} \tag{2.11}$$

These two vectors are clearly linearly dependent, indicating that we only have one constraint, and we can proceed with the first vector. There is no unique way to impose the constraint, and we finally end up with the following Γ matrix:

$$\hat{\mathbf{\Gamma}}_2'' = \begin{pmatrix} 1 & -2 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & -2 & 0 \\ 1 & 2 & 1 & -2 & 0 & -2 \end{pmatrix}.$$

The last step checks if the translation group removes any of the rows by constructing the matrix $\hat{\mathcal{V}}_2$ and the first row would be removed because it turns out to be a vector of all zeros at the level of the lattice.

Therefore, the final monomial representation matrix has two rows and could be written as follows:

$$\hat{\mathbf{\Gamma}}_2''' = \begin{pmatrix} 1 & 0 & 1 & 0 & -2 & 0 \\ 1 & 2 & 1 & -2 & 0 & -2 \end{pmatrix}. \tag{2.12}$$

It's clear here that $\hat{\mathbf{\Gamma}}_2'''$ is not unique - let alone the choices one has when enforcing homogeneity of free space, one could also transform it by any invertible linear transform without modifying the physics.

Thus, the final potential at second order is as follows:

$$V^{(2)} = \sum_{\mathbf{R}_a} \mathbf{\Phi}_2 \hat{\mathbf{\Gamma}}_2''' \xi^{(2)}_{\mathbf{R}_a}. \tag{2.13}$$

The label $\mathbf{\Psi}$ is changed to $\mathbf{\Phi}$ in order to denote that we are working with the fully irreducible expansion coefficients where all of the symmetry requirements have been built in. As indicated by the change in the shape of Γ, the number of parameters is reduced from 6 to 2 when symmetries are being built in.

The preceding outline shows how a symmetrized monomial representation could be built, though there is still a large degree of flexibility in how to implement it. When moving to more complex scenarios, it would be favorable if one has an approach that can more naturally utilize symmetry from the beginning instead of directly working with the monomial representation. In particular, it would be useful to write the identity representations as tensor products of symmetric variables, i.e. symmetric atomic

displacement modes, which inherently respect the homogeneity of free space; and this gives rise to the slave mode expansion sketched in Sec. 2.2 in a general case.

Before giving a formal presentation of the slave mode expansion, it is worth illustrating it in a trivial example. One could start by forming the symmetrized atomic displacement modes from $\{u_{\bar{1}}, u_0, u_1\}$ and one choice of them that transform like the irreducible representations of C_2 is given as follows:

$$\phi_{B^{(1)}} = u_0 \qquad \phi_A = u_1 - u_{\bar{1}} \qquad \phi_{B^{(2)}} = u_1 + u_{\bar{1}} \tag{2.14}$$

The mode that is not orthogonal to a uniform shift would be removed, as this would violate homogeneity of free space. In this case, this mode corresponds to a linear combination of both B modes, and removing it leaves us with the following two modes:

$$\phi_B = u_1 - 2u_o + u_{\bar{1}} \qquad \phi_A = u_1 - u_{\bar{1}} \tag{2.15}$$

These variables already satisfy homogeneity of free space, and they transform like irreducible representations of the point group so it is clear that there are two terms at second order that transform like the identity: ϕ_A^2 and ϕ_B^2. One can construct the matrix $\hat{\mathcal{V}}^{(2)}$ to demonstrate that the translation group does not remove any products, and then one has the irreducible potential:

$$\begin{aligned}
V^{(2)} &= \sum_{\mathbf{R}_a} \mathbf{\Phi}'_2 \begin{pmatrix} \phi_A^2 \\ \phi_B^2 \end{pmatrix} \\
&= \sum_{\mathbf{R}_a} \mathbf{\Phi}'_2 \begin{pmatrix} 1 & 0 & 1 & 0 & -2 & 0 \\ 1 & 4 & 1 & -4 & 2 & -4 \end{pmatrix} \xi^{(2)}_{\mathbf{R}_a} \\
&= \sum_{\mathbf{R}_a} \mathbf{\Phi}'_2 \begin{pmatrix} 1 & 0 & 1 & 0 & -2 & 0 \\ 2 & 4 & 2 & -4 & 0 & -4 \end{pmatrix} \xi^{(2)}_{\mathbf{R}_a} \\
&= \sum_{\mathbf{R}_a} \mathbf{\Phi}_2 \begin{pmatrix} 1 & 0 & 1 & 0 & -2 & 0 \\ 1 & 2 & 1 & -2 & 0 & -2 \end{pmatrix} \xi^{(2)}_{\mathbf{R}_a}
\end{aligned}$$

where we have expressed the potential in the monomial representation, shifted the second row by the first row of $\hat{\mathbf{\Gamma}}''_2$, reduced it again by a factor of 2, demonstrating the equivalence to equation 2.13.

The interpretation in this simple case is quite straightforward: given next-nearest neighbor coupling at quadratic order, one simply has a nearest neighbor spring and a next-nearest-neighbor spring.

2.4 Slave Mode Expansion

In general, the slave mode expansion for a potential is a series of identities built from bottom up instead of from top down using a set of symmetric variables ϕ that, as mentioned before, satisfy homogeneity of free space. These variables will be called *slave modes* hereafter. The slave mode expansion has all symmetry constraints built in and its number of parameters will be reduced because of it.

2.4.1 Slave Modes

In this section, the derivation of slave modes will be introduced. Though there is a wide degree of flexibility in choosing the slave modes, the optimum choice depends on the material and the use of the method. Here a typical scenario is outlined, and specific cases will be dealt with later.

1. Determine a cluster of atoms for which the anharmonic terms will be included. This cluster will be associated with a given unit cell (typically primitive), though it could contain atoms which are outside of the unit cell. *At least two atoms must be present in the chosen cluster*. We will refer to this as the slave cluster.

2. A center of highest symmetry and its point group should be identified for the chosen cluster. Each atom in the cluster has d degrees of freedom, where d is the dimension of space. Then the representation formed by these atomic displacements could be decomposed into the irreducible representations as a new set of vectors.

3. d linearly independent, symmetrized vectors that correspond to a uniform shift of the cluster need to be eliminated as they would violate homogeneity of free space; the rest are orthogonalized to them. The remaining vectors of modes are the *slave modes*, and they can essentially be thought of as molecular entities. The slave mode representation then comprises irreducible representations they transform like.

4. All non-translation space group operations should be used to determine if translationally inequivalent slave clusters are generated – the identities as the same combination of slave mode products from different slave clusters will be combined as a new identity for the lattice. This will be shed light on in Sec. 2.5.3.

5. The translation group may then be used to generate all translationally equivalent sets.

It may be useful to have multiple types of slave clusters associated with each unit cell (as labeled by s in Sec. 2.4.3), and then the above procedures will be executed for each slave cluster. This will indeed be the case for PbTe.

At this point, we have created a set of variables that respect all of the necessary symmetries, and the tensor product of these variables is a particular realization of the generic monomial representation that was presented in section 2.3. It should be noted that the slave modes are not simply a change of basis, as they have a higher dimension than degrees of freedom in the crystal, which could be viewed as enlarging the dimensionality of the system. If one wanted to use the slave modes as independent variables, then a constraint would have to be satisfied in order to be sure that the vibrational state is physical. In other words, an arbitrary vector in the space of slave modes will not necessarily have a corresponding vector in the space of displacements. However, this poses no problem in this work as we will always be using the slave modes as dependent variables. One can directly recover equation 2.1 by simply expanding the products of slave modes in equation 2.17.

2.4.2 Identities

The symmetric product determines how many linearly independent identity representations are contained in the product space of given irreducible representations. In essence, one can easily construct the characters for the symmetric product representation of a generic representation at a given order and the characters determine the number of identity representations. In this chapter we consider up to fourth order, and the characters for the symmetric product of a given representation are given as follows for second, third, and fourth orderZhou and Pulay (1989):

$$\begin{aligned}
\chi_2(R) &= \frac{1}{2}\left[\chi(R)^2 + \chi(R^2)\right] \\
\chi_3(R) &= \frac{1}{6}\left[\chi(R)^3 + 3\chi(R^2)\chi(R) + 2\chi(R^3)\right] \\
\chi_4(R) &= \frac{1}{24}\left[\chi(R)^4 + 8\chi(R)\chi(R^3) + 3\chi(R^2)^2\right. \\
&\qquad \left. +6\chi(R)^2\chi(R^2) + 6\chi(R^4)\right]
\end{aligned} \tag{2.16}$$

where R is an element of the group and $\chi(R)$ is the character of R in the given representation.

We will denote the direct product using the notation $\otimes$ and the symmetric product as $\odot$ hereafter. If one is dealing with the symmetric product of a single irreducible representation, the general formulas in equation 2.16 can be directly applied. For example, if we are considering the O_h point group and a quartic term $E_g \odot E_g \odot E_g \odot E_g$, the above equation reveals that this yields the direct sum $2E_g \oplus A_{1g}$, and therefore there is only one nonzero expansion coefficient. It is useful to note that one can even more rapidly deduce an upper limit on the number of expansion coefficients by considering the direct product $E_g \otimes E_g \otimes E_g \otimes E_g = 5E_g \oplus 3A_{2g} \oplus 3A_{1g}$, as the symmetric product is a subset of the direct product. This allows one to quickly determine if there are any nonzero projections. In the case of products with multiple types of irreducible representations, or different instances of the same irreducible representation, the symmetric product may be replaced by the direct product. These simple rules are all that is needed. Given that our slave modes already transform like irreducible representations, it is trivial to know *a-priori* how many nonzero coefficients a given product will have. Once the number of identities is determined, the projection operator can be used to construct them in that subspace.

2.4.3 Expansion

Therefore, the slave mode expansion for potential could be written down as follows:

$$\begin{aligned} V = & \sum_{\mathbf{R}s} \sum_{\alpha i} \Phi^{s}_{\alpha} \, \phi^{(i)}_{\alpha \mathbf{R}s} \phi^{(i)}_{\alpha \mathbf{R}s} \\ & + \sum_{\mathbf{R}s} \sum_{\substack{\alpha\beta\gamma \\ \zeta,ijk}} \Phi^{s\zeta}_{\alpha\beta\gamma} \Theta^{\zeta,ijk}_{\alpha\beta\gamma} \, \phi^{(i)}_{\alpha \mathbf{R}s} \phi^{(j)}_{\beta \mathbf{R}s} \phi^{(k)}_{\gamma \mathbf{R}s} \\ & + \sum_{\mathbf{R}s} \sum_{\substack{\alpha\beta\gamma\delta \\ \zeta,ijkl}} \Phi^{s\zeta}_{\alpha\beta\gamma\delta} \Theta^{\zeta,ijkl}_{\alpha\beta\gamma\delta} \, \phi^{(i)}_{\alpha \mathbf{R}s} \phi^{(j)}_{\beta \mathbf{R}s} \phi^{(k)}_{\gamma \mathbf{R}s} \phi^{(l)}_{\delta \mathbf{R}s} + \cdots \end{aligned} \tag{2.17}$$

In this expansion, $\alpha, \beta, \gamma, \delta$ label irreducible representations and i, j, k, l label the row of irreducible representations since they could be more than one dimensional. In addition, $\mathbf{R}$ is a lattice vector and s labels a cluster associated with a given unit cell. Therefore, the slave modes ϕs are atomic displacement modes within the atomic cluster labeled by s in the primitive cell translated by $\mathbf{R}$ and transform like the superscript row of the subscript irreducible representations of its point group. It should be noted

that cross terms between the clusters with different $\mathbf{R}$ or s are not written as their contribution can be accounted for by simply including larger clusters. On the other hand, the combination of $\alpha, \beta, \gamma, \delta$ could label a product space of the associated irreducible representations. Since there could be more than one identity representation within the corresponding symmetric product representation (see Sec. 2.4.2), their coefficients Φ will be differentiated by ζ. Last but not least, Θ, the Clebsch-Gordan (CG) coefficients, which is a group theoretical construct and is independent of any particular application, states the projection of the ζth identity on each of the basis of the product spaceRykhlinskaya and Fritzsche (2006).

The quadratic terms in this expansion are diagonal because only self-products of irreducible representations at second order contain identity. While we have explicitly written out the quadratic terms using slave modes, we will assume that these will normally be obtained using traditional approaches to compute phonons. For higher orders, the identities derived within a product space could always be written down as a summation of its projection on the basis of the space, indicating that one could directly read the CG coefficients from the identities after they are generated by applying the projection operator. In addition, Sec. 2.4.2 shows that symmetric product operation gives the number of linearly independent identities within a given product space, therefore one could apply the projection operator on a few of the basis to obtain all the linearly independent identities and a phase convention will be needed to show which ones of the basis are used to generate the final set of identities; ours will be introduced in Chapter 3.

2.4.4 Some Examples of Symmetric Products Using 4th Order Irreducible Representations in Oh Point Group

The following examples show how to derive the number of linearly independent identities given some 4th order product of irreducible representations in Oh point group by applying the aforementioned symmetry product rules.

$$Eg \odot Eg \odot Eg \odot Eg = A1g \oplus 2Eg \tag{2.18}$$

$$T2u \odot T2u \odot T2u \odot T2u = 2A1g \oplus 2Eg \oplus T1g \oplus 2T2g \tag{2.19}$$

$$
\begin{aligned}
&2T1u \odot 2T1u \odot 2T1u \odot 2T1u \\
&\quad =(T1u \oplus T1u') \odot (T1u \oplus T1u') \odot (T1u \oplus T1u') \odot (T1u \oplus T1u') \\
&\quad =(T1u \odot T1u \odot T1u \odot T1u) \oplus (T1u \otimes (T1u' \odot T1u' \odot T1u')) \oplus \\
&\quad\quad (T1u' \otimes (T1u \odot T1u \odot T1u)) \oplus ((T1u \odot T1u) \otimes (T1u' \odot T1u')) \\
&\quad =2(T1u \odot T1u \odot T1u \odot T1u) \oplus 2(T1u \otimes (T1u' \odot T1u' \odot T1u')) \oplus \\
&\quad\quad (T1u \odot T1u) \otimes (T1u' \odot T1u') \\
&\quad =2(2A1g \oplus 2Eg \oplus T1g \oplus 2T2g) \oplus 2(T1u \otimes (A2u \oplus 2T1u \oplus T2u)) \oplus \\
&\quad\quad (A1g \oplus Eg \oplus T2g) \otimes (A1g \oplus Eg \oplus T2g) \\
&\quad =(4A1g \oplus 4A1g \oplus 3A1g \oplus ...) \\
&\quad =11A1g \oplus ...
\end{aligned}
\tag{2.20}
$$

$$
\begin{aligned}
&Eg \odot Eg \odot T2g \odot T2g \\
&\quad =(Eg \odot Eg) \otimes (T2g \odot T2g) \\
&\quad =(A1g \oplus Eg) \otimes (A1g \oplus Eg \oplus T2g) \\
&\quad =2A1g \oplus ...
\end{aligned}
\tag{2.21}
$$

$$
\begin{aligned}
&T1g \odot T1g \odot T2g \odot T2g \\
&\quad =(T1g \odot T1g) \otimes (T2g \odot T2g) \\
&\quad =(A1g \oplus Eg \oplus T2g) \otimes (A1g \oplus Eg \oplus T2g) \\
&\quad =3A1g \oplus ...
\end{aligned}
\tag{2.22}
$$

$$
\begin{aligned}
&T1g \odot T1g \odot 2T1u \odot 2T1u \\
&\quad =(T1g \odot T1g) \otimes (2T1u \odot 2T1u) \\
&\quad =(T1g \odot T1g) \otimes ((T1u \oplus T1u') \odot (T1u \oplus T1u')) \\
&\quad =(T1g \odot T1g) \otimes (2(T1u \odot T1u) \oplus T1u \otimes T1u') \\
&\quad =(A1g \oplus Eg \oplus T2g) \otimes (2(A1g \oplus Eg \oplus T2g) \oplus (A1g \oplus Eg \oplus T1g \oplus T2g)) \\
&\quad =(A1g \oplus Eg \oplus T2g) \otimes (3A1g \oplus 3Eg \oplus 3T2g \oplus T1g) \\
&\quad =9A1g \oplus ...
\end{aligned}
\tag{2.23}
$$

$$
\begin{aligned}
&T2g \odot T2g \odot 2T1u \odot T2u \\
&\quad =2(T2g \odot T2g \odot T1u \odot T2u) = 2(T2g \odot T2g) \otimes T1u \otimes T2u \\
&\quad =2(A1g \oplus Eg \oplus T2g) \otimes T1u \otimes T2u \\
&\quad =2(T1u \oplus (T1u \oplus T2u) \oplus (A2u \oplus Eu \oplus T1u \oplus T2u)) \otimes T2u \\
&\quad =2(2T2u \oplus ...) \otimes T2u \\
&\quad =4A1g \oplus ...
\end{aligned}
\tag{2.24}
$$

$$
\begin{aligned}
&Eg \odot T1g \odot T1g \odot T2g \\
&\quad =Eg \otimes (T1g \odot T1g) \otimes T2g = Eg \otimes (A1g \oplus Eg \oplus T2g) \otimes T2g \\
&\quad =(Eg \oplus (A1g \oplus A2g \oplus Eg) \oplus (T1g \oplus T2g)) \otimes T2g \\
&\quad =(T2g \oplus ...) \otimes T2g \\
&\quad =A1g \oplus ...
\end{aligned}
\tag{2.25}
$$

$$
\begin{aligned}
&A1g \odot T2g \odot 2T1u \odot 2T1u \\
&\quad =A1g \otimes T2g \otimes (2T1u \odot 2T1u) \\
&\quad =A1g \otimes T2g \otimes (T1u \odot T1u \oplus T1u \otimes T1u' \otimes T1u' \odot T1u') \\
&\quad =A1g \otimes T2g \otimes (2(T1u \odot T1u) \oplus T1u \otimes T1u') \\
&\quad =A1g \otimes T2g \otimes (2(A1g \oplus Eg \oplus T2g) \oplus (A1g \oplus Eg \oplus T1g \oplus T2g)) \\
&\quad =A1g \otimes T2g \otimes (3T2g \oplus ...) \\
&\quad =3A1g \oplus ...
\end{aligned}
\tag{2.26}
$$

$$
\begin{aligned}
&T1g \odot T1g \odot T1g \odot T2g \\
&\quad =(T1g \odot T1g \odot T1g) \otimes T2g \\
&\quad =(A2g \oplus 2T1g \oplus T2g) \otimes T2g \\
&\quad =A1g \oplus ...
\end{aligned}
\tag{2.27}
$$

$$
\begin{aligned}
&2T1u \odot T2u \odot T2u \odot T2u \\
&\quad =2(T1u \odot T2u \odot T2u \odot T2u) \\
&\quad =2(T1u \otimes (T2u \odot T2u \odot T2u)) \\
&\quad =2(T1u \otimes (A1u \oplus T1u \oplus 2T2u)) \\
&\quad =2A1g \oplus ...
\end{aligned}
\tag{2.28}
$$

$$
\begin{aligned}
&2T1u \odot 2T1u \odot 2T1u \odot T2u \\
&\quad =(2T1u \odot 2T1u \odot 2T1u) \otimes T2u \\
&\quad =((T1u \oplus T1u') \odot (T1u \oplus T1u') \odot (T1u \oplus T1u')) \otimes T2u \\
&\quad =((T1u \odot T1u \odot T1u) \oplus (T1u \odot T1u' \odot T1u') \oplus (T1u \odot T1u \odot T1u') \\
&\qquad \oplus (T1u' \odot T1u' \odot T1u')) \otimes T2u \\
&\quad =(2(T1u \odot T1u \odot T1u) \oplus 2(T1u \odot T1u' \odot T1u')) \otimes T2u \\
&\quad =(2(A2u \oplus 2T1u \oplus T2u) \oplus 2(T1u \otimes (A1g \oplus Eg \oplus T2g))) \otimes T2u \\
&\quad =2((A2u \oplus 2T1u \oplus T2u) \oplus (T1u \otimes (A1g \oplus Eg \oplus T2g))) \otimes T2u \\
&\quad =2((A2u \oplus 2T1u \oplus T2u) \\
&\qquad \oplus (T1u \oplus T1u \oplus T2u \oplus A2u \oplus Eu \oplus T1u \oplus T2u)) \otimes T2u \\
&\quad =2(3T2u \oplus ...) \otimes T2u \\
&\quad =6A1g \oplus ...
\end{aligned}
\tag{2.29}
$$

2.5 Slave Mode Expansion for the $2d$ Square Lattice

To show how slave mode expansion works we apply it here in a two-dimensional square lattice with one atom per unit cell. We will explore the square cluster for slave modes, and a dimer cluster would also be addressed.

2.5.1 Square Cluster

A square cluster contains (see Fig. 2.1) 4 atoms in the two dimensional square lattice and its point symmetry group is C_{4v}Cornwell (1997). The representation of the atomic displacements in the square cluster is eight dimensional and can be decomposed as $\Gamma = A_1 \oplus A_2 \oplus B_1 \oplus B_2 \oplus 2E$ (see figure 2.1 top panel). In this case the E irreducible representation appears twice. One set of the E irreducible representations could be chosen to be shifts of the cluster while the other set could be orthogonalized to these shifts via a linear transformation. Therefore, the E representation corresponding to a shift would be removed (as indicated by the red X in figure 2.1), and the remaining slave mode representation will be $A_1 \oplus A_2 \oplus B_1 \oplus B_2 \oplus E$.

As discussed before, the second order identities could only be self-products, or diagonal since the product table says that only $A_1 \otimes A_1$, $A_2 \otimes A_2$, $B_1 \otimes B_1$, $B_2 \otimes B_2$ and $E \otimes E$ contain A_1. Therefore, at second order there will be the following products that not only satisfy the homogeneity of free space but also transform as identity: $\phi^2_{A_1}, \phi^2_{B_1}, \phi^2_{A_2}, \phi^2_{B_2}, \phi^2_{E^{(1)}} + \phi^2_{E^{(2)}}$. The last one could be achieved by applying the projection operator on either $\phi^2_{E^{(1)}}$ or $\phi^2_{E^{(2)}}$ (applying the projection operator on $\phi_{E^{(1)}}\phi_{E^{(2)}}$ results in zero). Next, all such products that overlap with a given cluster (see Fig. 2.1 bottom panel for an illustration) must be summed over in order to construct $\hat{\mathcal{V}}_2$:

$$\frac{1}{4}\begin{pmatrix} 2 & 2 & -2 & -1 & -1 & 2 & -1 & \dots \\ 2 & 2 & -2 & -1 & 1 & 2 & -1 & \dots \\ 2 & -2 & 2 & -1 & 1 & 2 & -1 & \dots \\ 2 & -2 & 2 & -1 & -1 & 2 & -1 & \dots \\ 4 & -4 & -4 & 2 & 0 & 4 & 2 & \dots \end{pmatrix} \begin{pmatrix} x_2^2 \\ x_2x_3 \\ x_2x_1 \\ x_2x_0 \\ x_2y_0 \\ x_3^2 \\ x_3x_1 \\ \vdots \end{pmatrix}, \tag{2.30}$$

and the linearly dependent identities could be removed. In essence, the rank of $\hat{\mathcal{V}}_2$ is 4 and that indicates that one of the products $\phi^2_{A_1}, \phi^2_{B_1}, \phi^2_{A_2}, \phi^2_{B_2}$ is linearly dependent and could be removed. Finally, there remains 4 nonzero expansion coefficients, as well as 4 linearly independent identities at quadratic order, corresponding to the following products: $\phi^2_{A_1}, \phi^2_{B_1}, \phi^2_{B_2}, \phi^2_{E^{(1)}} + \phi^2_{E^{(2)}}$.

A potential as a series of these identities therefore automatically satisfies point symmetry and homogeneity of free space. What's more, since any lattice symmetry operation could be decomposed into a point symmetry operation and a lattice vector translation, with symmetry incorporated within a cluster and any other clusters within the lattice being a replication and translation of it, lattice symmetry is also satisfied.

2.5.2 Clebsh Gordan Coefficients

The Clebsh Gordan Coefficients could be read directly from the identities after they are generated; they could be normalized or not, as one could apply any linear transformation to Γ. We will be showing the CG coefficients for identities up to 4th order in this square lattice example.

Since we have achieved all quadratic terms, the Clebsh Gordan Coefficients could

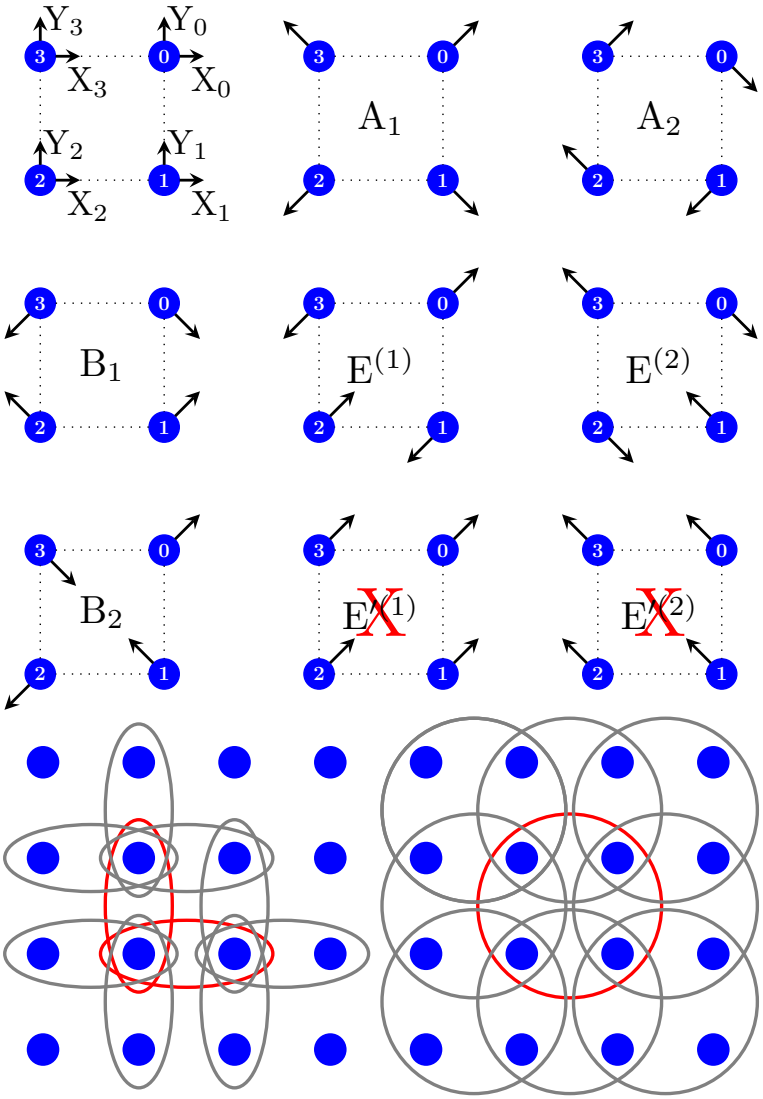

Figure 2.1: (Top panel) Normal modes for the square cluster in the square lattice. (Bottom panel) A schematic illustrating the summation of overlapping slave modes for the case of the dimer (left) and the square cluster (right). The slave clusters for a central unit cell are illustrated in red while translationally shifted.

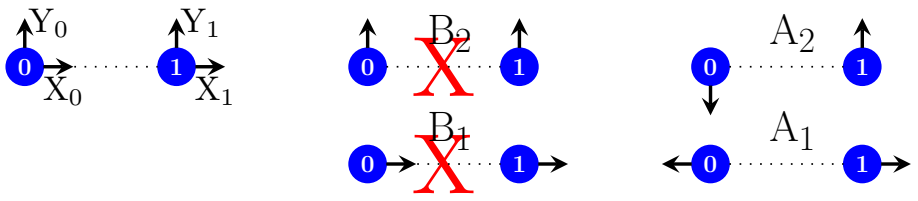

Figure 2.2: Normal modes for the dimer cluster in the square lattice.

be written down directly: $\Theta^{1,11}_{EE} = \Theta^{1,22}_{EE} = \Theta^{2,11}_{B_2B_2} = \Theta^{3,11}_{B_1B_1} = \Theta^{4,11}_{A_1A_1} = \Theta^{5,11}_{A_2A_2} = 1$. They are diagonal.

Third order terms could be achieved by applying the projection operator on basis of the product spaces of irreducible representations containing identity. For example, $B_2 \otimes E \otimes E$ contains A_1, applying the projection operator on each of the basis spanning this product space - $\phi_{B_2\mathbf{R}s}(\phi^{(1)}_{E\mathbf{R}s})^2$, $\phi_{B_2\mathbf{R}s}(\phi^{(2)}_{E\mathbf{R}s})^2$ and $\phi_{B_2\mathbf{R}s}\phi^{(1)}_{E\mathbf{R}s}\phi^{(2)}_{E\mathbf{R}s}$ - gives a linearly independent identity: $\phi_{B_2\mathbf{R}s}(\phi^{(1)}_{E\mathbf{R}s})^2$ - $\phi_{B_2\mathbf{R}s}(\phi^{(2)}_{E\mathbf{R}s})^2$. Therefore, its CG coefficients are $\Theta^{1,111}_{B_2EE} = 1$ and $\Theta^{1,122}_{B_2EE}$ = -1. The other terms could be achieved similarly and give $\Theta^{2,111}_{A_2B_1B_2} = 1$, $\Theta^{3,111}_{A_1A_2A_2} = 1$, $\Theta^{4,111}_{A_1B_2B_2} = 1$, $\Theta^{5,112}_{A_2EE} = 1$, $\Theta^{6,111}_{A_1A_1A_1} = 1$, $\Theta^{7,111}_{A_1EE} = \Theta^{7,122}_{A_1EE} = 1$ and $\Theta^{8,111}_{A_1B_1B_1} = 1$.

Fourth order could be achieved in the same way. For example, $A_2 \otimes B_1 \otimes E \otimes E$ contains A_1, and applying the projection operator on each of the basis spanning this product space- $\phi_{A_2\mathbf{R}s}\phi_{B_1\mathbf{R}s}(\phi^{(1)}_{E\mathbf{R}s})^2$, $\phi_{A_2\mathbf{R}s}\phi_{B_1\mathbf{R}s}(\phi^{(2)}_{E\mathbf{R}s})^2$ and $\phi_{A_2\mathbf{R}s}\phi_{B_1\mathbf{R}s}\phi^{(1)}_{E\mathbf{R}s}\phi^{(2)}_{E\mathbf{R}s}$ - gives one linearly independent identity: $4\phi_{A_2\mathbf{R}s}\phi_{B_1\mathbf{R}s}(\phi^{(1)}_{E\mathbf{R}s})^2$ - $4\phi_{A_2\mathbf{R}s}\phi_{B_1\mathbf{R}s}(\phi^{(2)}_{E\mathbf{R}s})^2$; its CG coefficients will therefore be $\Theta^{1,1111}_{A_2B_1EE} = 4$ and $\Theta^{1,1122}_{A_2B_1EE}$ = -4. The other identity terms could be achieved similarly and their CG coefficients are $\Theta^{2,1111}_{B_1B_1EE} = 4$ and $\Theta^{2,1122}_{B_1B_1EE} = 4$, $\Theta^{3,1111}_{A_1A_1A_1A_1} = 8$, $\Theta^{4,1111}_{EEEE} = 4$ and $\Theta^{4,2222}_{EEEE} = 4$, $\Theta^{5,1111}_{A_2A_2EE} = 4$ and $\Theta^{5,1122}_{A_2A_2EE} = 4$, $\Theta^{6,1111}_{B_1B_1B_1B_1} = 8$, $\Theta^{7,1111}_{A_1B_2EE}$ = -4 and $\Theta^{7,1122}_{A_1B_2EE} = 4$, $\Theta^{8,1111}_{A_1A_1A_2A_2} = 8$, $\Theta^{9,1111}_{B_2B_2EE} = 4$ and $\Theta^{9,1122}_{B_2B_2EE} = 4$, $\Theta^{10,1111}_{A_2A_2A_2A_2} = 8$, $\Theta^{11,1111}_{A_1A_1EE} = 4$ and $\Theta^{11,1122}_{A_1A_1EE} = 4$, $\Theta^{12,1111}_{A_1A_1B_1B_1} = 8$, $\Theta^{13,1111}_{A_2A_2B_1B_1} = 8$, $\Theta^{14,1111}_{A_2A_2B_2B_2} = 8$, $\Theta^{15,1112}_{A_1A_2EE} = 8$, $\Theta^{16,1111}_{B_2B_2B_2B_2} = 8$, $\Theta^{17,1111}_{A_1A_2B_1B_2} = 8$, $\Theta^{18,1111}_{B_1B_1B_2B_2} = 8$, $\Theta^{19,1122}_{EEEE} = 8$, $\Theta^{20,1112}_{B_1B_2EE} = 8$ and $\Theta^{21,1111}_{A_1A_1B_2B_2} = 8$.

2.5.3 Primer on Dimer

One could further consider a slave cluster of two nearest-neighbor atoms (i.e. dimer cluster) (see figure 2.2), and it has point group C_{2v}Cornwell (1997). The representation

for the dimer cluster is four dimensional and can be decomposed as $\Gamma = A_1 \oplus A_2 \oplus B_1 \oplus B_2$ (see figure 2.1 top panel). The two normal modes $B_1 \oplus B_2$ correspond to uniform shifts of the cluster, and therefore these modes will be removed, as indicated by the red X, leaving only $A_1 \oplus A_2$. There will therefore be two slave mode products at second order for both the horizontal dimer and vertical dimer: $\phi^2_{A_1}$ and $\phi^2_{A_2}$. If one simply writes down the potential following the procedures on square cluster and label the two dimer types using different s, lattice symmetry would not be preserved – the vertical and horizontal dimers that are symmetrically identical in the lattice are not in the potential. To preserve that, one needs to merge the two types of dimers into one and its associated new identities will be the summations of the corresponding ones from the merged dimers. This is exactly what step 4 means in the construction of slave modes.

Chapter 3

Methods

In the last chapter, we introduced the slave mode expansion as a series of identities. In this chapter, we will start with a discussion on how the generation of identities could be realized in linear algebra. On the other hand, the identities need to be parameterized before the expansion could really function as a true potential. Thus, we would also introduce the operations and numerical methods, i.e. finite difference and singular value decomposition, that realizes it.

3.1 Identity Generation

As mentioned in the last chapter, the projection operator is applied to each of the basis of the product space of given irreducible representations that contains them, therefore the product space of collections of slave modes with each collection containing those that transform like rows of a given irreducible representation, to generate the identities and keep those that are linearly independent. One would therefore need to define a phase convention to label the basis – so that the identities could be reproduced efficiently thereafter. In our program, we go through all rows of the last irreducible representation before we move on to change the rows of the previous one and etc and the basis went through earlier will be labeled a smaller number. The number used in labeling starts from 1. For example, the basis of $E \otimes E$ would be labeled as follows: $\phi_{E^{(1)}}\phi_{E^{(1)}} - 1$, $\phi_{E^{(1)}}\phi_{E^{(2)}} - 2$, $\phi_{E^{(2)}}\phi_{E^{(1)}} - 3$ and $\phi_{E^{(2)}}\phi_{E^{(2)}} - 4$.

3.1.1 Projection Operator

The general projection operator is defined to be $\sum_T \chi^{*(p)}(T)\hat{\mathbf{O}}_\mathbf{T}$ with χs being the character numbers of a given representation and $\hat{\mathbf{O}}_\mathbf{T}$ being the symmetry opera-

torCornwell (1997). The identity representation has all character number being one, therefore, the projection operator for identity would be $\sum_T \hat{\mathbf{O_T}}$. For slave modes that transform like rows of an irreducible representation, it is straightforward to apply $\hat{\mathbf{O_T}}$, as one could write down the slave modes as vectors in the same space where $\hat{\mathbf{O_T}}$ is a matrice. However, for the products of slave mode, one has to be careful. In our program, we apply one of the $\hat{\mathbf{O_T}}$s on each of the slave mode in the product and compute the tensor product of the results every time. The products will then be summed up as a candidate for final identities after all of the $\hat{\mathbf{O_T}}$s have been applied. For instance, $\sum_T \hat{\mathbf{O_T}}(\phi_A \otimes \phi_B) = \sum_T (\hat{\mathbf{O_T}}\phi_A) \otimes (\hat{\mathbf{O_T}}\phi_B)$

In details, the slave modes are written down as vectors in the space of atomic displacements within a chosen slave cluster, where the symmetry operators are written down as matrices. Therefore, applying the operations on a slave mode simply becomes a matrix multiplication. One could also perform a linear transformation on the atomic displacement space so that the symmetry operation matrices become block diagonalized and the slave mode vectors become the new basis of this rotated space.

When all the identities have been generated using the projection operator, being vectors in the slave mode product space they could be further written down as vectors in the product space of atomic displacements. Therefore, one could pick out the linearly independent ones by stacking them up in a matrice and screening for those that increase the rank of this matrice.

3.1.2 $\mathcal{V}$ Matrices

One not only needs to pick out the linearly independent identities from all the candidates generated within a slave cluster, but also needs to make sure that they are still linearly independent at the level of the lattice. The former has already been realized in the last section, and the latter would be achieved via the construction of $\mathcal{V}$ matrices.

To construct the $\mathcal{V}$ matrices, matrices stacked up by the vectors of linearly independent identities are built within a chosen slave cluster and other ones that overlap with it and summed up. When building up the identities in the overlapping slave clusters, one could actually copy the vectors in the atomic displacement product space within the chosen one but relabel its basis. The vectors could then be written down as scalars and transformed back into a set of different vectors in the original atomic displacement product space – and the matrices stacked up by such vectors could be summed up directly.

3.2 Identity Parameterization: Coefficient Mapping

After the identities are achieved, the next step is to parameterize for their coefficients; we will call them slave mode coefficients. In general, there are many approaches to compute them. An obvious approach would be to construct a large data set of distorted structures in the anharmonic regime and compute the corresponding energies and forces using DFT; the dataset may then be used to fit the coefficients using standard procedures. The drawback of such an approach is that one is always faced with the problems of overfitting or including data that is beyond the order of current model. While there are standard statistical methods to address such problems, we believe other approaches are likely more straightforward. Another approach would be to compute individual expansion coefficients for given monomials (ie. equation 2.1), analogous to what is done for the harmonic case in phonons, and map them into the slave mode coefficients as they should be related. In fact, the computed monomial coefficients are only of limited use given that numerical errors will prevent them from satisfying all the necessary symmetries. However, the linear relation between the slave mode coefficients and the monomial coefficients (see equation 3.1 for an example) which forms matrices mapping the monomial coefficients to slave mode coefficients at each order such that the slave mode coefficients are uniquely defined enforces all symmetry constraints. While it would be desirable to directly compute the slave mode coefficients, this is not straightforward as the slave modes are not orthogonal to each other.

The matrices mapping the monomial coefficients to the slave mode coefficients could be formed as follows. Because each identity could be written down as a series of monomials, for each monomial ever appeared, its coefficient could be achieved using those of the identities containing them. For example, in the slave mode expansion achieved in Sec. 2.5.1, all of the linearly independent identities at quadratic order contain x_2^2 – $\phi_{A_1}^2$, $\phi_{B_1}^2$, $\phi_{B_2}^2$ contain $\frac{1}{4} \times 2$ of it while $\phi_{E^{(1)}}^2 + \phi_{E^{(2)}}^2$ contains $\frac{1}{4} \times 4$ of it. Therefore, if the slave mode coefficients -Φs- are determined, the coefficient of x_2^2 ($\Psi_{x_2x_2}$) could also be achieved and it would be $\frac{1}{4}(2\Phi_{A_1} + 2\Phi_{B_1} + 2\Phi_{B_2} + 4\Phi_E)$. The coefficients of other monomials ever appeared in the identities could also be calculated in the same way and one could come up with the following mapping matrice in the

equation:

$$\frac{1}{4}\begin{pmatrix} 2 & 2 & 2 & 4 \\ 2 & 2 & -2 & -4 \\ -2 & -2 & 2 & -4 \\ -1 & -1 & -1 & 2 \\ -1 & 1 & -1 & 0 \\ 2 & 2 & 2 & 4 \\ -1 & -1 & -1 & 2 \\ \vdots & \vdots & \vdots & \vdots \end{pmatrix} \begin{pmatrix} \Phi_{A_1} \\ \Phi_{B_1} \\ \Phi_{B_2} \\ \Phi_E \end{pmatrix} = \begin{pmatrix} \Psi_{x_2x_2} \\ \Psi_{x_2x_3} \\ \Psi_{x_2x_1} \\ \Psi_{x_2x_0} \\ \Psi_{x_2y_0} \\ \Psi_{x_3x_3} \\ \Psi_{x_3x_1} \\ \vdots \end{pmatrix}. \tag{3.1}$$

This linear equation maps monomial coefficients back into slave mode coefficients. Therefore, one could compute monomial coefficients such that their number is larger than or equal to that of slave mode coefficients, or equivalently, the number of linearly independent rows of the above matrix is greater than or equal to the number of columns; and the slave mode expansion could be uniquely defined. This linear equation is then solved by Singular Value DecompositionWilliam H. Press (2007); Zaki and Wagner Meira (2014).

3.3 Numerical Methods

To compute the monomial coefficients, one could either use the $2N + 1$ theorem from density functional perturbation theoryGonze and Vigneron (1989); Debernardi *et al.* (1995); Deinzer *et al.* (2003), or a supercell approach using finite displacements could be used. We will opt for the latter in this thesis (see Sec. 3.3.2 for details). Considering the small errors within the numerical implementation of DFT and therefore those within monomial coefficients computed, the mapping matrices mentioned above should be preconditioned in practice so that the errors propagated from DFT to the slave mode coefficients could be minimized – this leads to the selection of an optimal set of monomials.

3.3.1 Condition Number

For a linear problem that solves Ax = b, to measure the propagated error from b to x, one uses the condition number of A. In essence, if the error in b is e, the error

propagated to the solution(x) from b is $||A^{-1}e||$ and the ratio of the relative error in x to the relative error in b is

$$\frac{||A^{-1}e||/||A^{-1}b||}{||e||/||b||} = (||A^{-1}e||/||e||) \cdot (||b||/||A^{-1}b||). \tag{3.2}$$

Its maximum value would be

$$\kappa(A) = ||A^{-1}|| \cdot ||A|| = \frac{\sigma_{max}(A)}{\sigma_{min}(A)}, \tag{3.3}$$

where $\sigma_{max}(A)$ and $\sigma_{min}(A)$ are maximal and minimal singular values of A respectively and $\kappa(A)$ is the condition number of Avan der Sluis (1969). Therefore, to reduce the propagated relative error, one needs to lower down $\kappa(A)$. Common approaches that decrease the condition number of a matrix include taking out of some of its rows without affecting its rank and scaling or equilibration of a matrixFarooq and Salhi (2011); Antia (2002). These apply to a general solution to a linear problem including Singular Value Decomposition.

In our case, we will be trying to minimize the condition number of the mapping matrice via row removal so that to reduce the propagated error from DFT. An "annealing" minimization approach would be taken. Every time one randomly picks a row whose removal does not affect the rank of the given matrice; if it decreases its condition number or doesn't increase that over a preset amount, it will be removed. One continues with this process before the condition number is stable or the number of trials exceeds a number that is large enough. From the construction process of the mapping matrice, we know we would also be removing the monomials related from all those that appear in the identities. Therefore, one finally ends up with an optimal set of monomials.

3.3.2 Finite Difference

The last essential part is to compute the monomial coefficients via a finite displacement approach. From the definition of Taylor series expansion, it is clear that the coefficients of a monomial in a potential is actually computable if one could achieve the value of the associated derivative. For example, if one targets at that of x_2^2 in the potential, it is actually $\frac{1}{2}\frac{\partial^2 E}{\partial x_2^2}$ with E being the system energy and therefore if one knows $\frac{\partial^2 E}{\partial x_2^2}$ one could compute it. On the other hand, any derivative value could be approximated using finite differenceLeVeque (2007). For instance, one could take a

central finite difference approach and the approximated value of the derivative would have the following mathematical expression –

$$\begin{aligned}
&\frac{\partial^n f}{\partial^h x_\alpha \partial^i x_\beta \partial^j x_\gamma \partial^k x_\delta}|_{x_\alpha=q_\alpha, x_\beta=q_\beta, x_\gamma=q_\gamma, x_\delta=q_\delta} = \\
&\frac{1}{(2\Delta)^n} \sum_{n_\alpha=0}^{h} \sum_{n_\beta=0}^{i} \sum_{n_\gamma=0}^{j} \sum_{n_\delta=0}^{k} \binom{h}{n_\alpha} \binom{i}{n_\beta} \binom{j}{n_\gamma} \binom{k}{n_\delta} \\
&(-1)^{n_\alpha+n_\beta+n_\gamma+n_\delta} f(q_\alpha + (h-2n_\alpha)\Delta, q_\beta + (i-2n_\beta)\Delta, \\
&q_\gamma + (j-2n_\gamma)\Delta, q_\delta + (k-2n_\delta)\Delta)
\end{aligned} \tag{3.4}$$

with q_α, q_β, q_γ and q_δ standing for atomic displacements, Δ being finite displacement and $n = h+i+j+k$. Therefore, the monomial coefficients could be achieved via finite difference, i.e. central finite difference, if one computes the values of energy functions appeared in the expression by imposing finite displacements and put them together. What's more, a derivative of energy could be derived from derivative of forces–

$$\begin{aligned}
\frac{\partial^n E}{\partial^h q_\alpha \partial^i q_\beta \partial^j q_\gamma \partial^k q_\delta} &= \frac{\partial^{n-1} F_\alpha}{\partial^{h-1} q_\alpha \partial^i q_\beta \partial^j q_\gamma \partial^k q_\delta} \\
&= \frac{\partial^{n-1} F_\beta}{\partial^h q_\alpha \partial^{i-1} q_\beta \partial^j q_\gamma \partial^k q_\delta} \\
&= \frac{\partial^{n-1} F_\gamma}{\partial^h q_\alpha \partial^i q_\beta \partial^{j-1} q_\gamma \partial^k q_\delta} \\
&= \frac{\partial^{n-1} F_\gamma}{\partial^h q_\alpha \partial^i q_\beta \partial^j q_\gamma \partial^{k-1} q_\delta},
\end{aligned} \tag{3.5}$$

implying that one could compute the values of force functions instead.

Error Tail of Central Finite Difference

We would then give a proof showing that the error tail of central finite difference approximation is a quadratic function of the finite displacement.

For a first order derivative, this is straightforward as

$$\begin{aligned}\frac{df}{dx}|_{x=x_0} &= \frac{f(x_0+\Delta)-f(x_0-\Delta)}{2\Delta} \\ &= [(f(x_0)+f'(x_0)\Delta+\frac{f^{(2)}(x_0)}{2!}\Delta^2-\frac{f^{(3)}(\xi)}{3!}\Delta^3) \\ &- (f(x_0)-f'(x_0)\Delta+\frac{f^{(2)}(x_0)}{2!}\Delta^2+\frac{f^{(3)}(\xi)}{3!}\Delta^3)]/2\Delta \\ &= f'(x_0)-\frac{f^{(3)}(\xi)}{3!}\Delta^2\end{aligned} \tag{3.6}$$

For a second order derivative, one could also apply the same steps and here we go

$$\begin{aligned}\frac{d^2f}{dx^2}|_{x=x_0} &= \frac{f'(x_0+\Delta)-f'(x_0-\Delta)}{2\Delta} \\ &= \frac{f(x_0+2\Delta)-f(x_0)-(f(x_0)-f(x_0-2\Delta))}{(2\Delta)^2} \\ &= \frac{f(x_0+2\Delta)+f(x_0-2\Delta)-2f(x_0)}{(2\Delta)^2} \\ &= [(f(x_0)+2f'(x_0)\Delta+4\frac{f^{(2)}(x_0)}{2!}\Delta^2-8\frac{f^{(3)}(x_0)}{3!}\Delta^3+16\frac{f^{(4)}(\xi)}{4!}\Delta^4) \\ &+ (f(x_0)-2f'(x_0)\Delta+4\frac{f^{(2)}(x_0)}{2!}\Delta^2+8\frac{f^{(3)}(x_0)}{3!}\Delta^3+16\frac{f^{(4)}(\xi)}{4!}\Delta^4) \\ &- 2f(x_0)]/(2\Delta)^2 \\ &= f^{(2)}(x_0)+8\frac{f^{(4)}(\xi)}{4!}\Delta^2\end{aligned} \tag{3.7}$$

In the above two cases, their quadratic tails stem from the facts that Δ^0 and Δ^2 terms for $\frac{df}{dx}$ on the numerator are cancelled out while Δ^0, Δ and Δ^3 terms for $\frac{d^2f}{dx^2}$ on the numerator are cancelled out. Therefore, one would wonder whether in general for an nth order derivative, Δ^η terms with $\eta = 0, 1, 2, ..., n-1, n+1$ on the numerator could be cancelled out so that the quadratic error tail for central finite difference becomes universal. We know for $\eta = 0, 1, 2, ..., n-1$, Δ^η terms must have been cancelled out by definition, therefore we only care about the case of $\eta = n+1$. The answer is yes and could be proven as follows.

From eqn. 3.4, it could be derived that the Δ^{n+1} terms on the numerator are

$$\sum_{n_\alpha=0}^{h}\sum_{n_\beta=0}^{i}\sum_{n_\gamma=0}^{j}\sum_{n_\delta=0}^{k}\sum_{a}\sum_{b}\sum_{c}\sum_{d}\binom{h}{n_\alpha}\binom{i}{n_\beta}\binom{j}{n_\gamma}\binom{k}{n_\delta}(-1)^{n_\alpha+n_\beta+n_\gamma+n_\delta} \\ ((h-2n_\alpha)\Delta)^a((i-2n_\beta)\Delta)^b((j-2n_\gamma)\Delta)^c((k-2n_\delta)\Delta)^d\frac{\partial^{n+1}f(q_\alpha,q_\beta,q_\gamma,q_\delta)}{\partial^a q_\alpha\partial^b q_\beta\partial^c q_\gamma\partial^d q_\delta}, \tag{3.8}$$

with the constraint that $a+b+c+d=n+1$ and $h+i+j+k=n$. Because of the difference in the partial derivative, one could separate different combinations of (a,b,c,d) and check if each of the terms could be zero – or whether the term

$$\sum_{n_\alpha=0}^{h}(-1)^{n_\alpha}\binom{h}{n_\alpha}((h-2n_\alpha)\Delta)^a\sum_{n_\beta=0}^{i}(-1)^{n_\beta}\binom{i}{n_\beta}((i-2n_\beta)\Delta)^b \\ \sum_{n_\gamma=0}^{j}(-1)^{n_\gamma}\binom{j}{n_\gamma}((j-2n_\gamma)\Delta)^c\sum_{n_\delta=0}^{k}(-1)^{n_\delta}\binom{k}{n_\delta}((k-2n_\delta)\Delta)^d \\ \frac{\partial^{n+1}f(q_\alpha,q_\beta,q_\gamma,q_\delta)}{\partial^a q_\alpha\partial^b q_\beta\partial^c q_\gamma\partial^d q_\delta}, \tag{3.9}$$

could be zero. If one looks at any of the sums individually, e.g. $\sum_{n_\alpha=0}^{h}(-1)^{n_\alpha}\binom{h}{n_\alpha}((h-2n_\alpha)\Delta)^a$, it would be found that it is 0 when a is 0 or symmetric otherwise – $n_\alpha=m$ component and $n_\alpha=h-m$ component yielding the same absolute value. In details, the $n_\alpha=m$ component is $(-1)^m\binom{h}{m}(h-2m)^a$ and the $n_\alpha=h-m$ component is $(-1)^{h-m}\binom{h}{m}(2m-h)^a=(-1)^{h+a-m}\binom{h}{m}(h-2m)^a$. What's more, no matter when h is even or odd, this holds because when h is even, the component in the middle is zero by definition – $n_\alpha=\frac{h}{2}$ and $h-2n_\alpha=0$. Therefore, one only concerns whether the symmetric components could be cancelled out.

This could be checked with a little bit more thoughts. When $h+a$ is even, $(-1)^m$ always have the same sign with $(-1)^{h+a-m}$, while when it is odd, they always have opposite signs. Thus, one could put all of the sums back into the product and it would be realized that the term would be zero if any of $h+a$, $i+b$, $j+c$ or $k+d$ is odd. Because the sum of them is $2n+1$ is odd, at least one of them is odd. Therefore, the term is zero and in fact each of the terms for different (a,b,c,d) combination should be zero and finally Δ^{n+1} terms are cancelled out.

Though a Δ^2 error tail is good enough for our work, one could further improve it using other finite differences that give rise to a higher order error tail. LeVeque (2007)

Optimal Δ

Since the error in approximation climbs with Δ quadratically according to the discussion above, one would choose a Δ that is small enough in an ideal case. Another intuitive reason why we do not prefer a Δ that is too large is that the function values there may lack information of the derivative where we are looking at. This would be it if the original data are perfect. However, in DFT, there is noise and one has to be careful. In essence, when Δ is too small, a prohibitive planewave cutoff and k-point mesh may be required to lower down the noise in the numerator but it might still be magnified a lot and therefore ruin the approximation – indicating that one would not prefer a Δ that is too small, either. Thus, the optimal Δ would usually be chosen to be somewhere in between for accuracy and efficiency. Examples would be shown when the method is applied in PbTe and Graphene.

Chapter 4

Application in PbTe

In this chapter, we will be applying the slave mode expansion to obtaining an ab-initio interatomic potential for PbTe. The potential will be expanded up to 4th order, with interaction constrained within an octahedron. It is then assessed in the way that it predicts the energy and stress, as well as phonon frequency under strain; and it is found that the potential works well up to substantial strains. A minimal model could also be achieved for the potential and it successfully reproduces its TO mode phonon splitting at Γ point under finite temperature.

4.1 PbTe and its TO Mode Phonon Splitting at Γ Point

PbTe is a three-dimensional material with rock-salt lattice structure with two atoms in one primitive cell – one Pb atom and the other Te atom. We will choose a primitive cell having vectors $a_1 = a/2(1,1,0)$, $a_2 = a/2(0,1,1)$ and $a_3 = a/2(1,0,1)$ (a = 6.5566$\mathring{A}$), with Pb atom at $(0,0,0)$ and Te atom at $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ (fractional coordinates). The point group symmetry of PbTe is O_h Leitsmann and Bechstedt (2010).

It has been found by inelastic neutron scattering (INS) that there are signatures of strong interactions in the temperature dependence of the phonon spectrum of PbTe, attracting significant attention to this system. For example, the most interesting behavior is observed at the zone center where the spectrum has remarkably split into two broad peaks under finite temperature, as measured in experimentsO. Delaire and Sales (2011); Jensen *et al.* (2012b) and shown in Fig. 4.1. However, theoretical works investigating them are scarce mainly because one cannot directly compute the temperature dependence of the phonon spectra for materials with appreciable phonon interactions within DFT. Since molecular dynamics provides another way around but one just needs an interatomic potential to carry it out efficiently, we are motivated to create one.

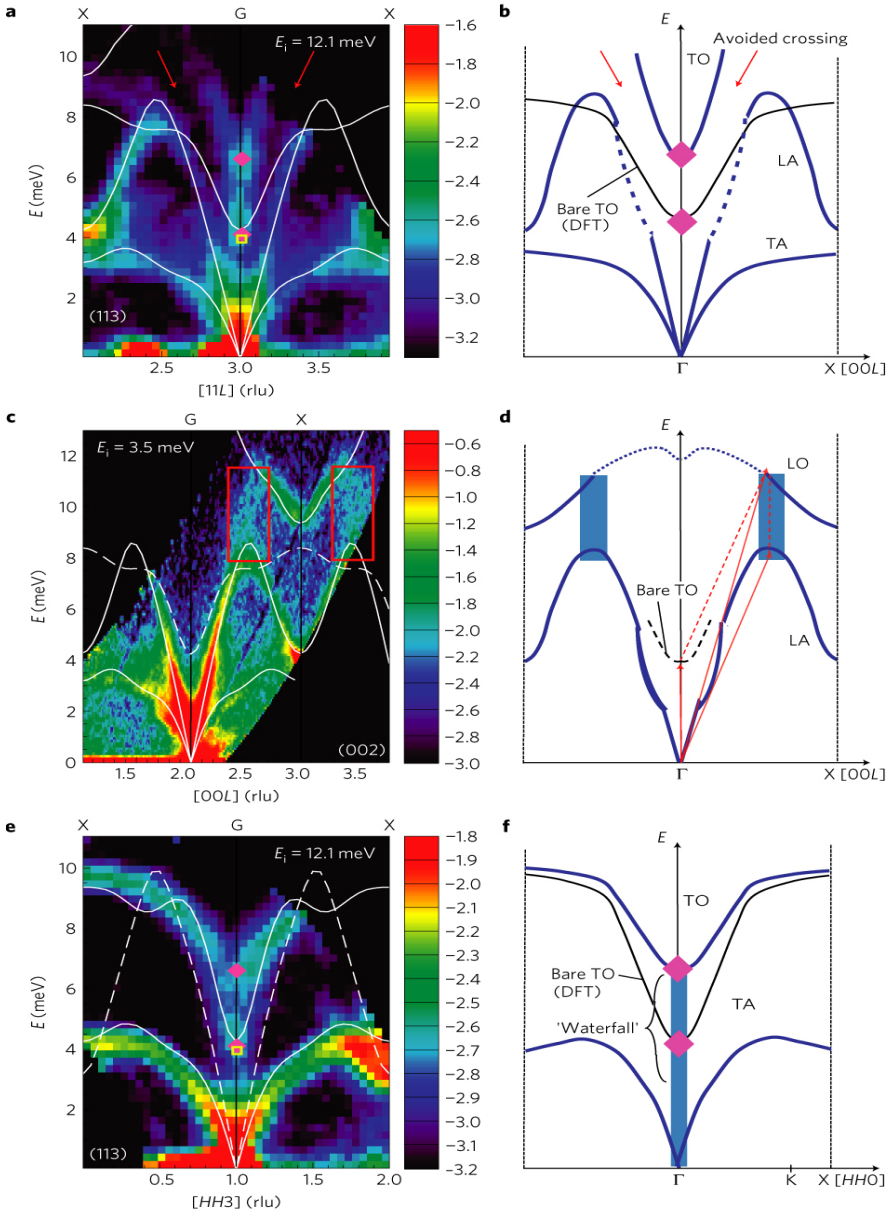

Figure 4.1: a,c,e, CNCS data for PbTe at 300K (logarithmic intensity scale), b,d,f, Schematic representations of the dispersions (blue lines), with blue rectangles representing diffuse extra scattering, and the bare TO branch as a thin black line. In all panels, pink diamonds indicate the positions of the peaks in the TO scans at Γ(113), obtained with HB3. The yellow square in a,e is ETO = 3.9±0.2 meV from ref. Cochran *et al.* (1966) (from paper O. Delaire and Sales (2011))

4.2 Group Theory Analysis

To construct the slave modes so that to expand the interatomic potential for PbTe, one starts with the selection of atomic cluster(s). There are two natural choices: the Pb-Te dimer and the octahedron (both Pb centered and Te centered). We will begin by considering the octahedron as the cluster of choice (see section 4.6 for the dimer), which implies that we will have anharmonic terms within next nearest neighbor for both Pb and Te. There will be two slave clusters associated with each primitive unit cell, each having O_h point symmetry, and these correspond to atoms connected with bold black lines in figure 4.2. Translationally equivalent clusters can be generated by shifting with the primitive lattice vectors (denoted as green lines in figure 4.2). We now proceed to decompose the displacement vectors into irreducible representations of the O_h point group, which would be $\Gamma = A_{1g} \oplus E_g \oplus T_{1g} \oplus T_{2g} \oplus 3T_{1u} \oplus T_{2u}$. However, one of the T_{1u}s is actually a mode that rigidly shifts the octahedron and should be removed based on the definition of slave mode which furthermore enforces the homogeneity of free space. Therefore, the slave mode representation of the displacement vectors within an Octahedron would be $\Gamma = A_{1g} \oplus E_g \oplus T_{1g} \oplus T_{2g} \oplus 2T_{1u} \oplus T_{2u}$, and they are shown in figure 4.3.

4.3 Slave Mode Expansion for PbTe

With slave modes derived, one could generate the slave mode expansion for PbTe by applying the projection operator on the basis of the product space of the slave modes. The harmonic terms will not be derived for the potential of PbTe since they could be computed using traditional approaches for computing phonons from first-principles, such as density functional perturbation theory or finite displacement supercell approaches. However, third and fourth order slave mode expansion terms will be derived. What's more, all of them will be achieved within two octahedra – one centered on Pb and the other centered on Te; they are shown in Fig. C.1 in Appendix C. Later in this chapter, one would see that a minimal model for the potential could be derived using slave modes within dimers - e.g. the two-atom cluster forming bond 01 in Fig. 4.3; these slave modes will be called dimer modes.

After forming the symmetric product representation in a given octahedron, showing that there are 29 nonzero products at third order and 153 nonzero products at fourth order. This will be the case for both Pb and Te centered octahedron. Nontranslational symmetry elements will not generate any translationally inequivalent slave clusters.

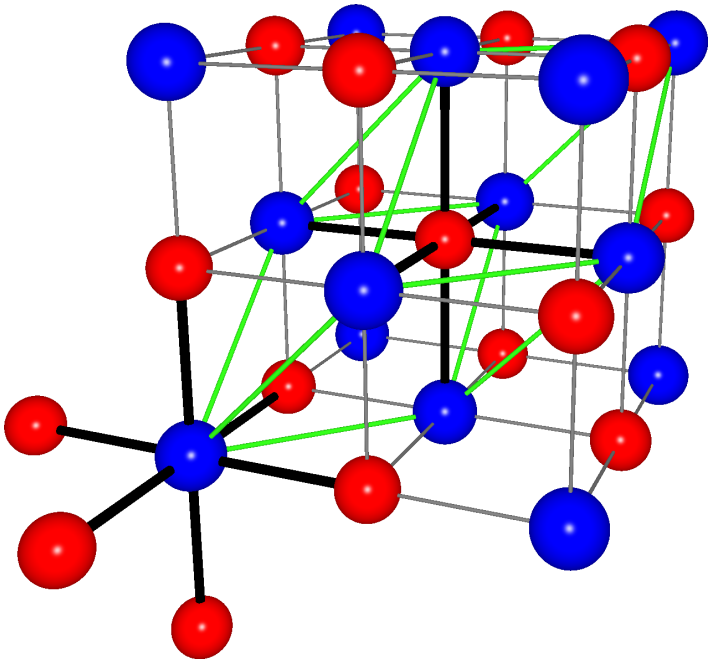

Figure 4.2: A section of the rock salt structure. The primitive unit cell is given in green. The two slave clusters associated with the primitive unit cell are denoted by atoms connected with bold lines.

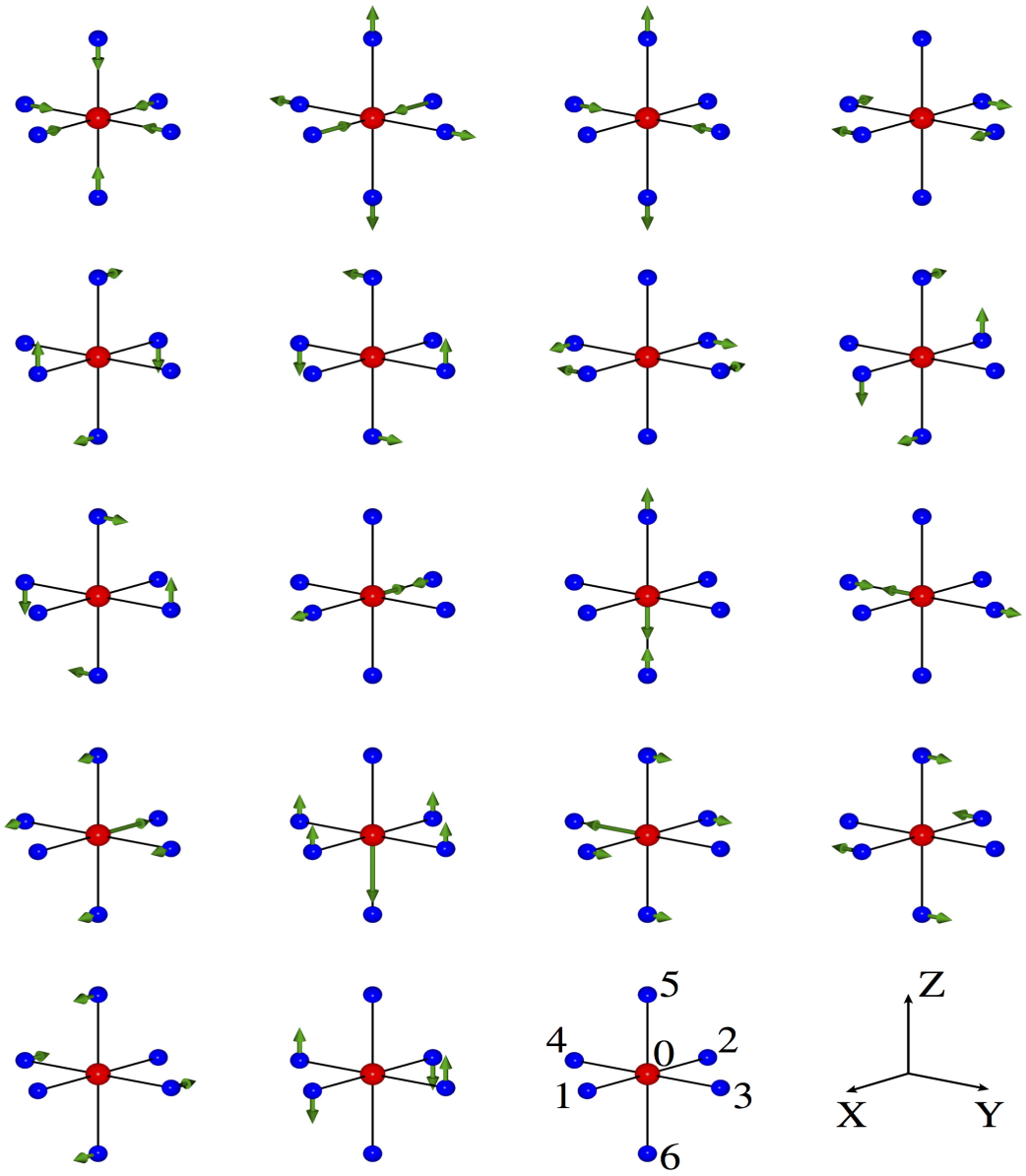

Figure 4.3: Octahedral modes transforming as the irreducible representations of the point group. The three T_{1u} modes which shift the octahedron have been removed. Reading from left to right and top to bottom, the modes are $A_{1g}, E_g, T_{1g}, T_{2g}, 2T_{1u}$, and T_{2u}. Our choice of coordinate system and numbering convention is given in the bottom right. Displacement vectors within a given mode have relative magnitudes of 1, 2, or 4, which can be identified by inspection.

Product	Phase	Pb-centered Φ	Te-centered Φ
$T_{2g} \otimes 2T_{1u} \otimes T_{2u}$	32, 45	-0.059,-0.048	-0.033,-0.043
$E_g \otimes T_{1g} \otimes T_{1g}$	1	-0.011	0.001
$T_{1g} \otimes T_{1g} \otimes T_{2g}$	16	0.002	-0.002
$A_{1g} \otimes E_g \otimes E_g$	1	0.074	-0.002
$T_{2g} \otimes 2T_{1u} \otimes 2T_{1u}$	38, 59, 84	-0.276,-0.245,-0.524	-0.129,-0.148,-0.284
$T_{1g} \otimes 2T_{1u} \otimes T_{2u}$	45, 54	0.102,-0.084	0.022,-0.025
$A_{1g} \otimes T_{2u} \otimes T_{2u}$	5	-0.01	N/A
$T_{2g} \otimes T_{2g} \otimes T_{2g}$	6	-0.003	0.002
$E_g \otimes 2T_{1u} \otimes T_{2u}$	20, 29	-0.041,0.067	0.008,0.001
$A_{1g} \otimes 2T_{1u} \otimes 2T_{1u}$	4, 15, 22	-1.849,1.288,0.635	-0.282,0.188,0.091
$E_g \otimes T_{2g} \otimes T_{2g}$	14	-0.003	-0.006
$T_{1g} \otimes 2T_{1u} \otimes 2T_{1u}$	6	-0.022	0.006
$E_g \otimes E_g \otimes E_g$	4	-0.035	0.005
$E_g \otimes 2T_{1u} \otimes 2T_{1u}$	4, 22, 51	-2.341,0.941,1.754	0.573,-0.197,-0.449
$T_{2g} \otimes T_{2u} \otimes T_{2u}$	2	0.002	-0.007
$E_g \otimes T_{1g} \otimes T_{2g}$	5	0.018	-0.005
$A_{1g} \otimes T_{2g} \otimes T_{2g}$	9	-0.002	0.006
$A_{1g} \otimes A_{1g} \otimes A_{1g}$	1	0.01	N/A
$A_{1g} \otimes T_{1g} \otimes T_{1g}$	1	-0.011	-0.004
$E_g \otimes T_{2u} \otimes T_{2u}$	10	0.008	0.003

Table 4.1: Nonzero third order products and the corresponding expansion coefficients. The second column indexes the basis of the product space which gives the identity after projection operator is applied. Terms designated N/A were those removed by the translation group.

Employing the translation group and constructing the matrices $\hat{\mathcal{V}}_3$ and $\hat{\mathcal{V}}_4$, one can demonstrate that some of the terms are redundant. In particular, two terms will be removed at third order, and four terms will be removed at fourth order. The final result is that there are 56 terms at third order and 302 terms at fourth order, for a total of 358 terms up to fourth order and within next-nearest neighbor range. The third order products, together with phase and corresponding coefficients are listed in table 4.1, while fourth order ones are listed in table 4.2; the phase convention is defined in Chapter 3 and how the coefficients are computed will be presented in Sec. 4.4. On the other hand, the CG coefficients we derived at the same time for all these terms are provided in Appendix E so that the terms could be conveniently reproduced.

Table 4.2: Nonzero fourth order products and the corresponding expansion coefficients. The second column indexes the basis of the product space which gives the identity after projection operator is applied. Terms designated N/A were those removed by the translation group.

Product	**Phase**	**Pb-centered Φ**	**Te-centered Φ**
$E_g \otimes E_g \otimes T_{2g} \otimes T_{2g}$	14, 32	-0.043, -0.034	0.008, 0.01
$T_{2g} \otimes T_{2g} \otimes 2T_{1u} \otimes T_{2u}$	83, 151, 36, 27	0.938, -0.681, 0.031, -0.05	-1.014, 0.742, 0.088, -0.077
$T_{2u} \otimes T_{2u} \otimes T_{2u} \otimes T_{2u}$	1, 5	0.017, 0.003	-0.015, 0.001
$E_g \otimes T_{1g} \otimes T_{1g} \otimes T_{2g}$	35	-0.0	0.003
$T_{1g} \otimes T_{1g} \otimes T_{1g} \otimes T_{2g}$	25	-0.007	-0.001
$A_{1g} \otimes T_{2g} \otimes T_{2g} \otimes T_{2g}$	6	0.001	0.002
$A_{1g} \otimes E_g \otimes T_{1g} \otimes T_{1g}$	14	0.029	-0.01
$T_{1g} \otimes T_{2g} \otimes T_{2g} \otimes T_{2g}$	9	-0.002	0.007
$E_g \otimes E_g \otimes T_{1g} \otimes T_{2g}$	14	-0.121	0.047
$2T_{1u} \otimes 2T_{1u} \otimes 2T_{1u} \otimes 2T_{1u}$	533, 1, 1044, 11, 22, 59, 606, 130, 15, 1037, 522	-8.18, 7.405, -3.203, 10.942, 45.45, -10.874, 13.284, -35.053, -2.019, 10.804, -28.53	17.113, 1.528, 7.597, -31.941, -10.505, 30.786, -31.418, 15.514, 7.908, -6.578, N/A
$T_{1g} \otimes T_{1g} \otimes T_{2g} \otimes T_{2g}$	73, 41, 11	0.003, 0.102, -0.005	0.0, -0.102, 0.003
$A_{1g} \otimes A_{1g} \otimes A_{1g} \otimes A_{1g}$	1	0.002	-0.001
$E_g \otimes T_{1g} \otimes T_{2g} \otimes T_{2g}$	47	0.002	0.005
$T_{2g} \otimes T_{2g} \otimes T_{2g} \otimes T_{2g}$	41, 5	0.017, 0.001	-0.017, -0.002
$T_{1g} \otimes T_{1g} \otimes T_{1g} \otimes T_{1g}$	41, 45	0.018, 0.003	-0.014, 0.001
$E_g \otimes T_{1g} \otimes 2T_{1u} \otimes T_{2u}$	54, 108, 1, 8	0.172, -0.297, 0.467, -0.001	-0.11, 0.195, -0.304, -0.006
$E_g \otimes T_{2g} \otimes 2T_{1u} \otimes 2T_{1u}$	89, 16, 146, 102	-1.391, 1.118, -0.416, 0.398	1.716, -0.56, 0.801, -0.685
$2T_{1u} \otimes T_{2u} \otimes T_{2u} \otimes T_{2u}$	18, 83	0.038, 0.054	-0.018, -0.018
$T_{1g} \otimes T_{1g} \otimes 2T_{1u} \otimes 2T_{1u}$	317, 53, 29, 95, 292, 152, 183, 155, 289	2.214, 0.136, 0.021, 0.089, -0.004, 0.833, 0.051, -2.914, -0.013	-1.801, -0.238, -0.05, -0.137, 0.092, -0.584, -0.107, 2.242, -0.046
$A_{1g} \otimes T_{2g} \otimes T_{2u} \otimes T_{2u}$	21	0.007	0.005
$E_g \otimes E_g \otimes E_g \otimes E_g$	4	0.024	-0.01
$E_g \otimes T_{1g} \otimes 2T_{1u} \otimes 2T_{1u}$	16, 192, 111, 167	1.062, 3.955, -2.932, -2.859	-0.674, -2.289, 1.606, 1.627
$A_{1g} \otimes T_{1g} \otimes T_{1g} \otimes T_{2g}$	8	-0.001	0.002
$T_{1g} \otimes T_{1g} \otimes T_{2u} \otimes T_{2u}$	77, 5, 12	0.006, 0.102, -0.005	0.001, -0.098, -0.002
$E_g \otimes T_{2g} \otimes 2T_{1u} \otimes T_{2u}$	17, 99, 71, 21	0.226, 0.207, -0.204, 0.248	-0.069, 0.098, 0.198, -0.363
$E_g \otimes E_g \otimes T_{1g} \otimes T_{1g}$	9, 28	0.071, -0.106	-0.026, 0.039
$A_{1g} \otimes T_{1g} \otimes 2T_{1u} \otimes T_{2u}$	10, 40	-0.263, -0.359	0.071, 0.118

$A_{1g} \otimes T_{2g} \otimes 2T_{1u} \otimes 2T_{1u}$	102, 38, 41	-0.905, 0.882, -1.902	0.675, -0.724, 1.459
$T_{1g} \otimes T_{1g} \otimes 2T_{1u} \otimes T_{2u}$	83, 39, 107, 74	0.986, -0.009, 0.025, -0.718	-0.918, 0.02, -0.027, 0.662
$E_g \otimes T_{2g} \otimes T_{2u} \otimes T_{2u}$	29	-0.003	0.002
$2T_{1u} \otimes 2T_{1u} \otimes 2T_{1u} \otimes T_{2u}$	30, 540, 280, 306, 142, 7	2.355, -1.842, -0.811, 4.857, -3.446, -1.88	-8.661, 4.674, 3.853, -10.649, 6.226, 4.979
$A_{1g} \otimes A_{1g} \otimes 2T_{1u} \otimes 2T_{1u}$	8, 11, 29	0.598, -0.725, 0.145	0.078, -0.158, 0.096
$A_{1g} \otimes E_g \otimes E_g \otimes E_g$	1	0.03	0.0
$A_{1g} \otimes E_g \otimes T_{2u} \otimes T_{2u}$	5	0.028	-0.005
$A_{1g} \otimes E_g \otimes T_{1g} \otimes T_{2g}$	10	0.17	-0.06
$A_{1g} \otimes E_g \otimes 2T_{1u} \otimes 2T_{1u}$	29, 54, 51	-2.974, -3.915, 2.377	0.315, 0.165, 0.021
$A_{1g} \otimes A_{1g} \otimes T_{1g} \otimes T_{1g}$	5	-0.018	0.001
$A_{1g} \otimes T_{1g} \otimes 2T_{1u} \otimes 2T_{1u}$	89	0.831	-0.347
$E_g \otimes E_g \otimes 2T_{1u} \otimes 2T_{1u}$	130, 47, 72, 11, 15 116	-0.093, -2.737, -0.91, -0.678, -0.85, 1.64	0.255, 0.112, -0.052, -0.397, 0.175, N/A
$A_{1g} \otimes A_{1g} \otimes T_{2g} \otimes T_{2g}$	1	-0.013	N/A
$A_{1g} \otimes T_{2g} \otimes 2T_{1u} \otimes T_{2u}$	10, 23	-0.146, -0.237	0.108, 0.16
$E_g \otimes E_g \otimes T_{2u} \otimes T_{2u}$	18, 36	0.043, -0.037	-0.009, 0.007
$A_{1g} \otimes E_g \otimes 2T_{1u} \otimes T_{2u}$	34, 20	0.754, -0.283	-0.344, 0.133
$T_{1g} \otimes T_{2g} \otimes 2T_{1u} \otimes T_{2u}$	83, 74, 22, 143, 155, 72, 79, 113	1.913, -1.372, -0.02, 0.04, -0.07, -0.004, -0.056, -0.026	-2.0, 1.461, -0.015, -0.052, 0.039, -0.027, 0.029, 0.038
$E_g \otimes T_{1g} \otimes T_{2u} \otimes T_{2u}$	2	-0.001	-0.001
$T_{2g} \otimes T_{2g} \otimes T_{2u} \otimes T_{2u}$	24, 77, 41	-0.001, 0.003, 0.098	-0.007, -0.002, -0.105
$2T_{1u} \otimes 2T_{1u} \otimes T_{2u} \otimes T_{2u}$	198, 99, 28, 264, 135, 72, 87, 20, 261	-0.194, -3.438, 0.63, 0.415, -0.47, 1.251, 0.813, 0.409, 2.36	0.326, 3.335, -0.834, 0.041, 0.531, -1.225, 0.133, 0.09, -2.28
$T_{2g} \otimes T_{2g} \otimes 2T_{1u} \otimes 2T_{1u}$	306, 196, 1, 317, 66, 8, 310, 162, 45	-2.88, -0.216, 0.857, 2.154, -0.093, -0.048, -0.015, 0.067, -0.118	2.73, -0.047, -0.8, -2.083, -0.056, -0.106, -0.125, 0.226, N/A
$T_{1g} \otimes T_{2g} \otimes 2T_{1u} \otimes 2T_{1u}$	15, 95, 120, 221, 18, 324, 117	3.295, -0.036, -0.071, -0.081, -7.9, -5.024, 0.104	-3.6, -0.228, -0.166, -0.148, 8.646, 5.441, 0.098
$A_{1g} \otimes A_{1g} \otimes T_{2u} \otimes T_{2u}$	1	-0.014	-0.0
$A_{1g} \otimes E_g \otimes T_{2g} \otimes T_{2g}$	9	0.018	-0.013
$T_{1g} \otimes T_{2g} \otimes T_{2u} \otimes T_{2u}$	60, 73	0.002, -0.202	-0.005, 0.205
$A_{1g} \otimes A_{1g} \otimes E_g \otimes E_g$	4	0.027	0.003
$E_g \otimes E_g \otimes 2T_{1u} \otimes T_{2u}$	6, 29	-0.288, -0.326	-0.008, 0.021

4.4 Computing Expansion Coefficients for PbTe

Having determined the slave mode expansion up to 4th order and within an Octahedron, the slave mode coefficients could now be computed. As described in Chapter 3, the monomial coefficients will be computed first and then mapped back to achieve the slave mode coefficients. The mapping matrices are preconditioned so that to reduce the propagation of noises from DFT runs to the slave mode coefficients; and this leads to the selection of a set of monomials. In our case of PbTe, we selected and computed 70 monomial coefficients at third order and 427 at fourth order.

4.4.1 DFT Runs and Finite Difference

As outlined in Chapter 3, the monomial coefficients are computed with finite difference and they are listed in Appendix D. Given that the forces are known from the Hellman-Feynman TheoremMartin (2008), the first derivatives will all be known for a given DFT computation. Using the central finite difference, one could then approximate higher order derivatives according to Eqn. 3.4.

VASP setup

The forces are computed within the framework of Density Functional Theory which is carried out using the generalized gradient approximation (GGA) by Perdew and WangPerdew *et al.* (1992) as implemented in the Vienna ab initio simulation package (VASP) Kresse and Hafner (1993, 1994); Kresse and Furthmuller (1996a,b); Kresse and Joubert (1999a). Gamma centered k-meshes depending on the supercell size are applied and a $3 \times 3 \times 3$ mesh is used for the smallest 64-atom supercell. Charge self-consistency is performed until the energy is converged to within 10^{-5} eV, and a plane wave cutoff of $175 - 350eV$ was used depending on the particular computation. Spin-orbit coupling was not utilized.

Optimal Δ for Finite Difference

In order to be sure the direct coefficients are robustly computed within finite difference, one must test for convergence with respect to the displacement size Δ in addition to the supercell size. If Δ is chosen to be too small, a prohibitive planewave cutoff and k-point mesh will be required, while if it is too large higher order terms will taint the computation. Therefore, there will be an optimum Δ which will be both efficient

and accurate, and this will strongly depend on the order of the derivative. In order to illustrate this point, the values of two different fourth order expansion coefficients are plotted as a function of Δ (see figure 4.4). A clear plateau emerges in both cases, revealing a robust value for Δ. After examining a wide range of different types of direct coefficients, we found that $\Delta = 0.01\mathring{A}$ is reliable for third order while $\Delta = 0.07\mathring{A}$ is reliable for fourth order.

Optimal Supercell Size for Finite Difference

Aside from choosing the optimal Δ for finite difference, one must also test for its convergence with respect to supercell size – to be sure that images are not interacting with one another. The minimum supercell dimension that was used was twice the conventional (ie. cubic) cell size, while the maximum was six times the conventional cell size. In order to illustrate this, we plot two fourth order coefficients as a function of unit cell size along a particular dimension (see figure 4.5), demonstrating that the changes in the coefficients are diminishing with increasing cell size. Our convergence criteria for supercell dimension was determined based on the largest finite difference coefficient at a specific order, and for third order the unit cell size was increased until changes were within 0.01 $eV/\mathring{A}^3$ while the threshold was $0.1eV/\mathring{A}^4$ for fourth order.

4.4.2 Slave Mode Expansion Coefficients

As mentioned in the beginning, we have computed 70 monomial coefficients at third order and 427 at fourth order. These numbers exceed the numbers of slave mode coefficients (56 at third order and 302 at fourth order), and therefore we have sets of overdetermined linear equations that uniquely determine the slave mode coefficients. Singular value decomposition is then used to find the optimum solution in terms of least squares and the final solutions for third and fourth order terms are plotted in Fig. 4.6. At third order, the Pb-centered slave modes have substantially larger coefficients than the Te-centered slave modes, while the differences are less pronounced for fourth order. On the other hand, the values of each slave mode coefficient have already been listed in Tables 4.1 and 4.2.

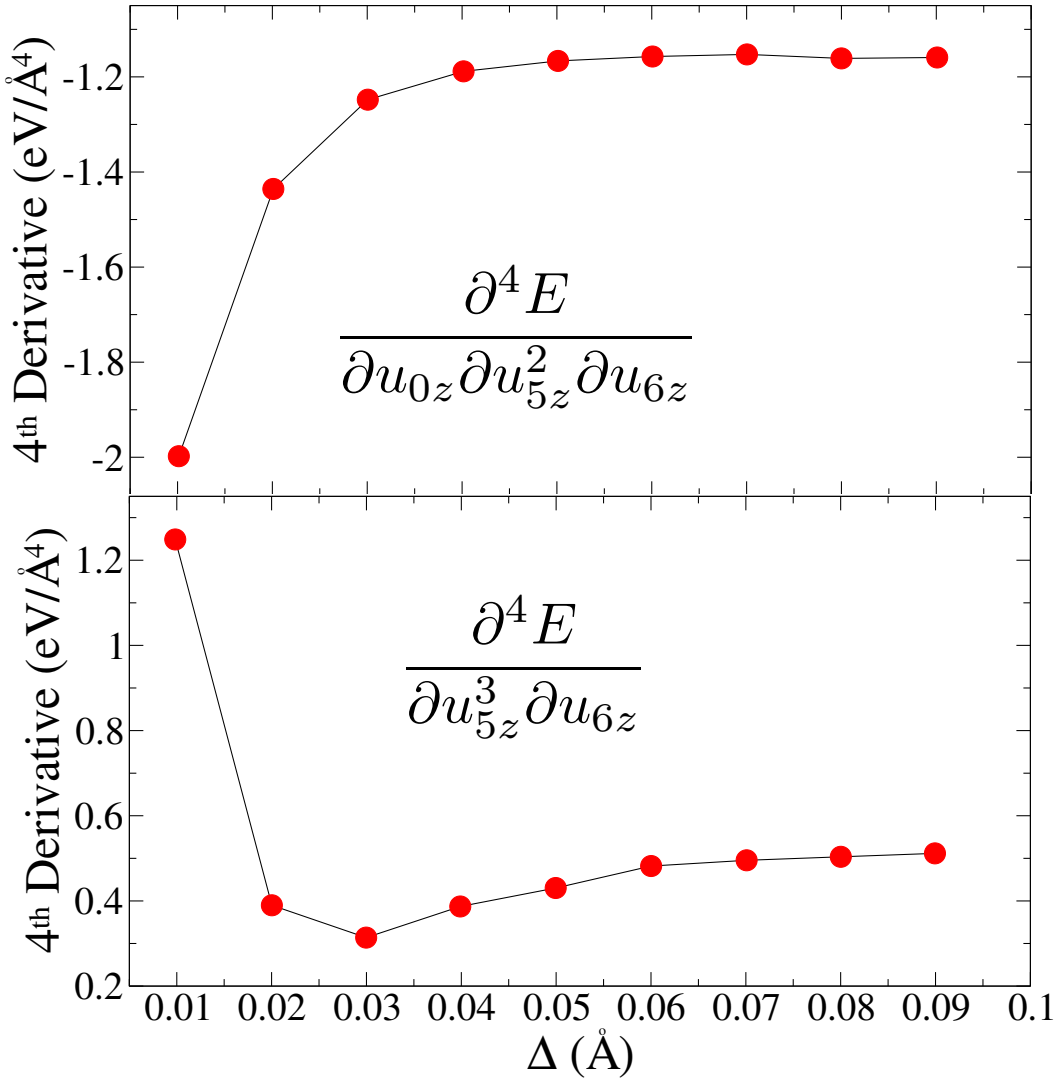

Figure 4.4: Fourth order derivatives computed using central step finite difference as a function of Δ for a conventional supercell choice of $2 \times 2 \times 3$ (ie. 96 atoms).

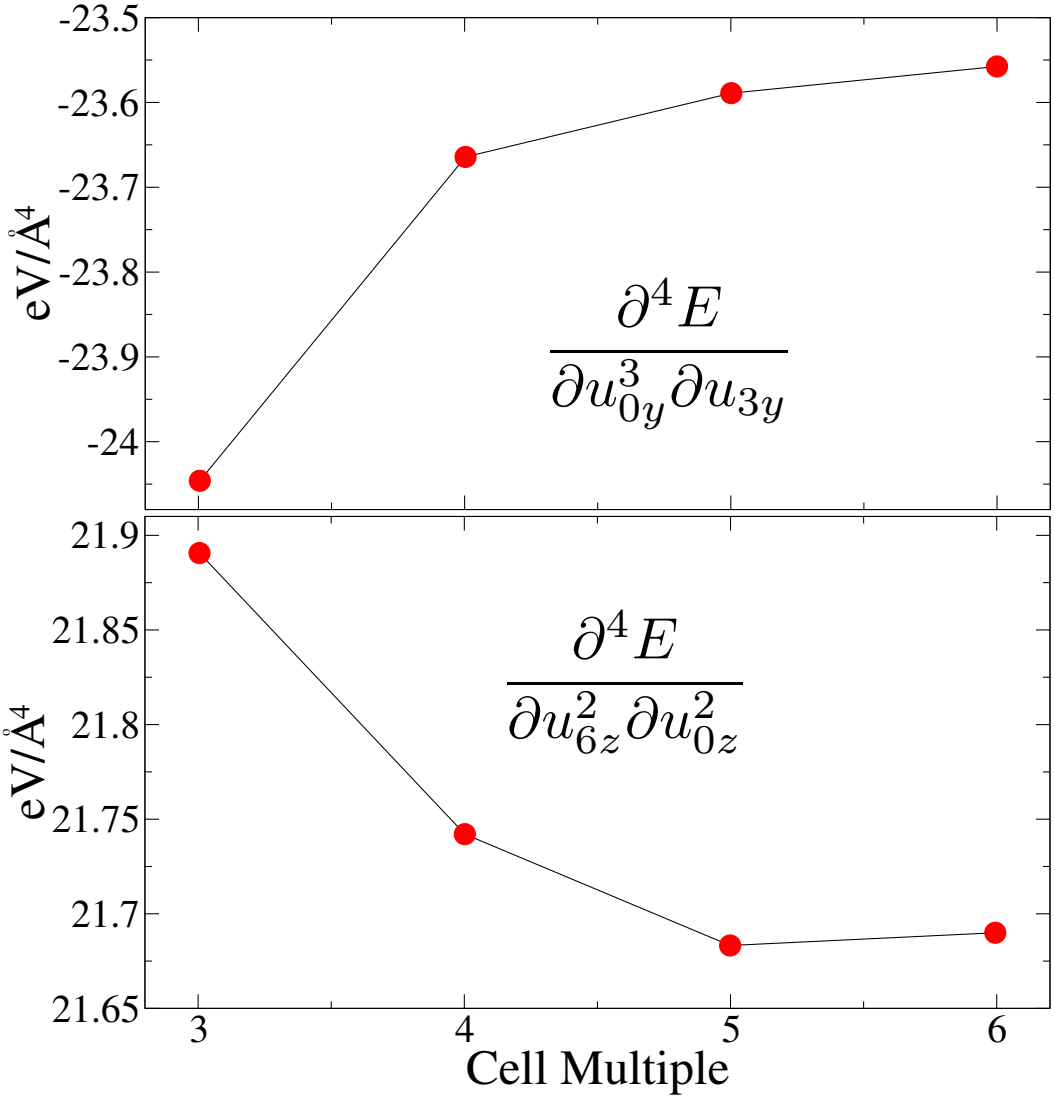

Figure 4.5: Fourth order derivatives computed using central step finite difference as a function of conventional supercell size in the y-direction (top panel) and the z-direction (bottom panel) for $\Delta = 0.07\mathring{A}$.

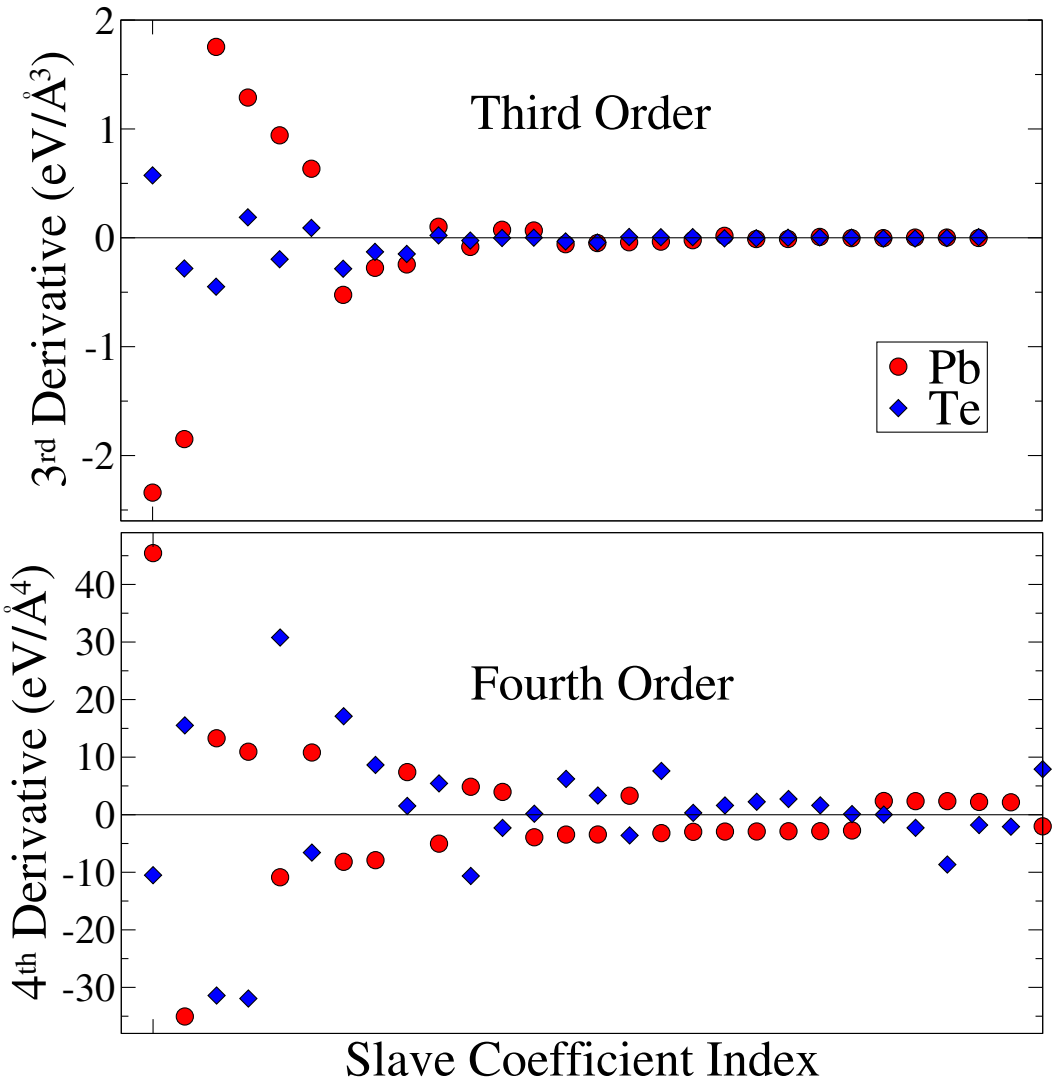

Figure 4.6: A plot of the third and fourth order slave mode product coefficients Φ. The values are ordered in decreasing magnitude for the Pb-centered coefficients, and the same absolute ordering is used for the Te-centered coefficients. Only a fraction of the fourth order terms are shown for clarity.

4.5 Assessing the Expansion

Having computed the slave mode expansion coefficients up to fourth order and within next nearest neighbor coupling, we now evaluate the overall reliability of our expansion. The major point of concern in the method we have employed to compute the slave mode coefficients is whether or not the slave mode expansion is sufficiently converged within the octahedron or if non-negligible terms beyond the octahedron are present. A potent test to address this issue is to use the slave mode expansion to compute energy, stress, and phonons as a function of lattice strain. It should be emphasized that our slave mode expansion is performed in the absence of any strain, but if our cluster is sufficiently large the expansion will be able to be used to compute the energetics under strain. Given that strain will amplify the coupling to long-range interactions, and that it is straightforward to compute the answer to these tests using DFT, this serves as an ideal testbed for any type of Taylor series expansion in terms of atomic displacements. PbTe is sufficiently polar such that there are long-range fields which will cause a non-negligible splitting of the optical modes near the Γ-point. These can be straightforwardly taken into account via Born effective chargesBaroni *et al.* (2001), but we do not include them in this study.

4.5.1 Energy and Stress under Strain

The first test is to compute the energy and the stress as a function of strain (see figure 4.7). As shown, there is remarkable agreement in the stress for strains as high as 7% and even higher for the energy. At 10% strain there is an error of roughly 8% in the stress. This favorable agreement suggests that longer range terms are not substantial.

4.5.2 Phonons under Strain

A more stringent test is to compute the phonons as a function of strain. We begin by computing the L-point phonons as a function of strain (see figure 4.8). As shown, there is remarkable agreement up to 5% strain.

Another test of phonons under strain is the Γ-point optical modes. This mode is of particular interest in the context of PbTe as it displays anomalous temperature dependenceJensen *et al.* (2012a); Delaire *et al.* (2011); Chen *et al.* (2014). We compute energy of the Γ-point optical modes as a function of triaxial, uniaxial, and shear strain (see figure 4.9). In the case of triaxial strain, the slave mode expansion precisely

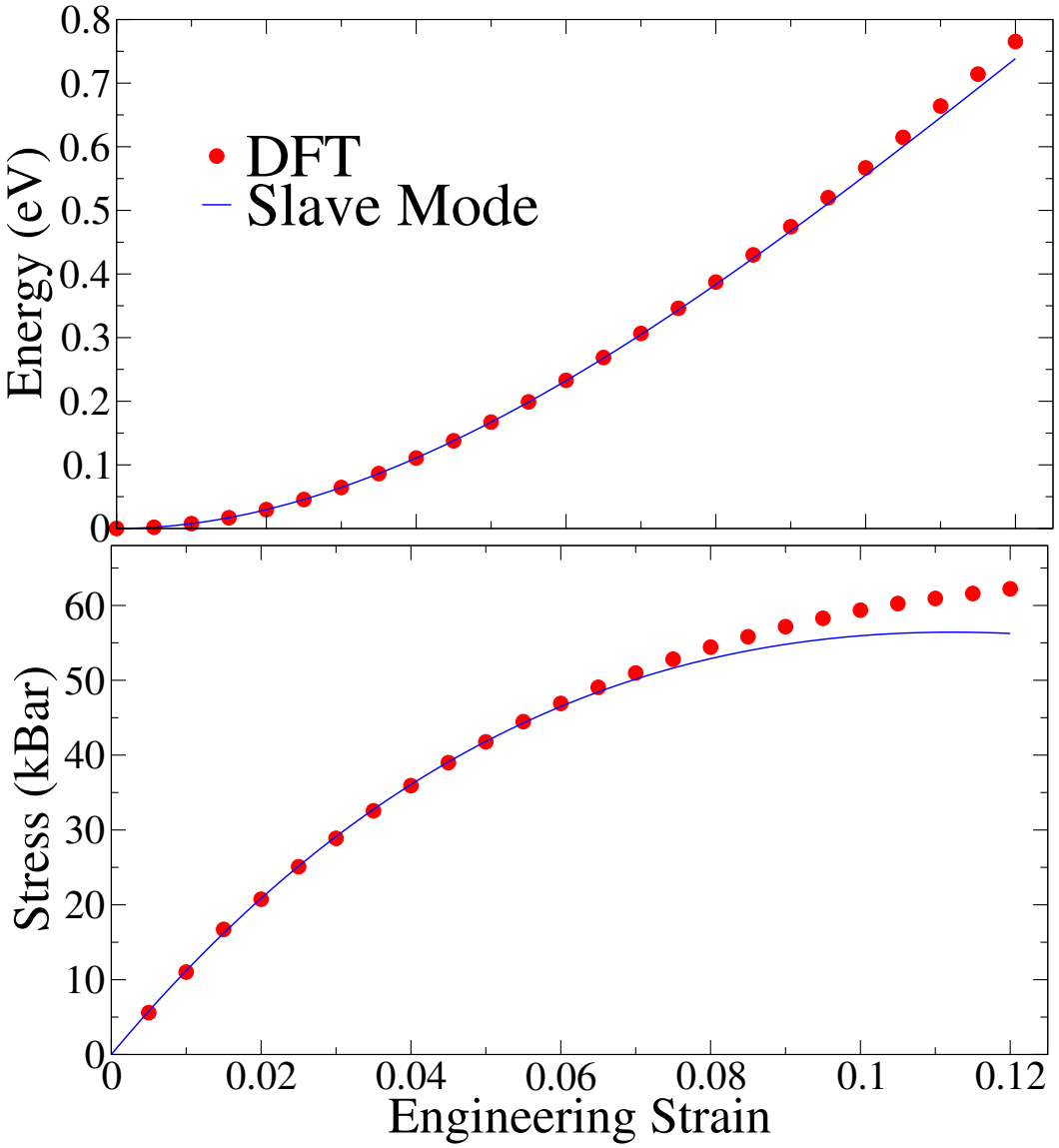

Figure 4.7: (Top Panel) Energy as a function of triaxial engineering strain. (Bottom Panel) True Stress as a function of triaxial engineering strain.

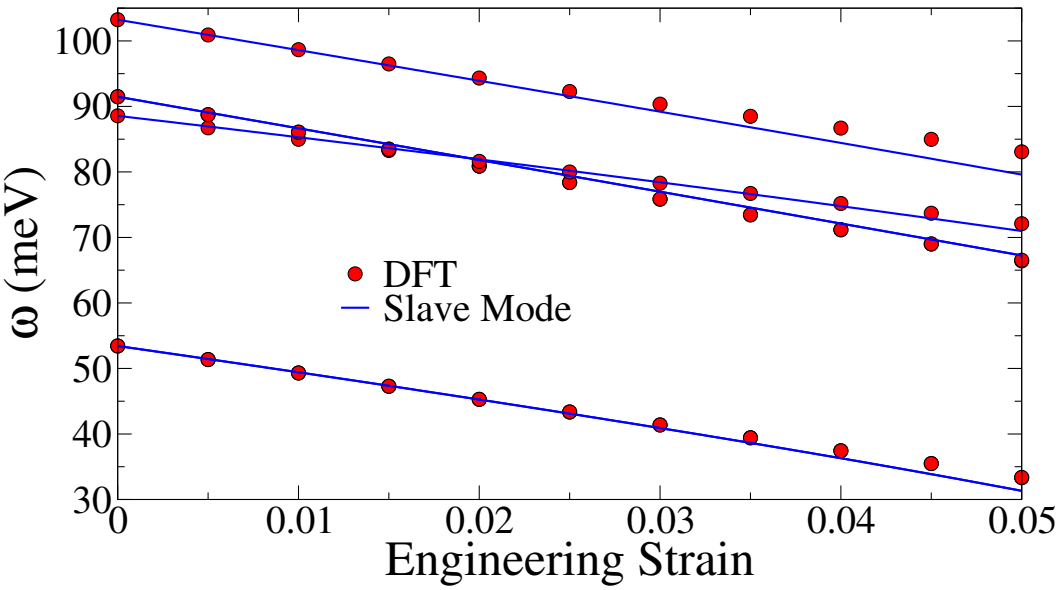

Figure 4.8: L-point phonon frequencies as a function of triaxial engineering strain.

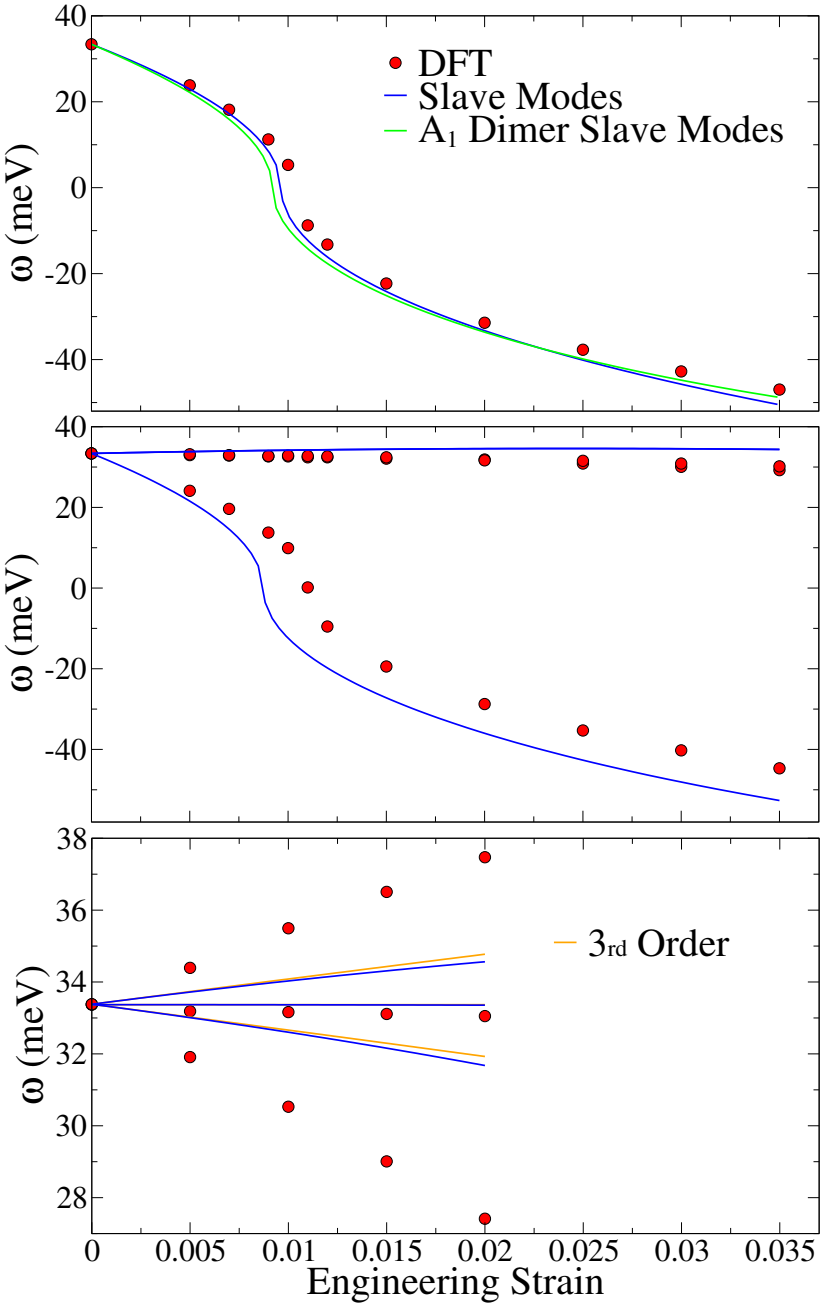

Figure 4.9: Γ-point optical phonon frequencies as a function of different engineering strain states: triaxial (top panel), uniaxial (middle panel), and shear γ_{xy} (bottom panel). In the top panel, the green curve uses the minimal slave mode expansion that has only two expansion coefficients. In the bottom panel, the orange curve uses only the third order slave mode terms.

captures the formation of a soft-mode. In the case of uniaxial strain, the slave mode expansion is highly accurate for small strains and properly captures the symmetry breaking of the optical modes. However, errors are apparent for the prediction of the soft mode at larger strains, though the error is relatively constant beyond 1.5%. In the case of shear strain, the splitting of the optical modes is underpredicted using the slave modes, though the error is still within reason in this range of strain. Nonetheless, the troubling aspect of this result is that it does not have the correct slope in the limit of small strains. Given that there is little difference in going from third to fourth order coefficients, this is likely a symptom of longer range terms that are not present in our expansion. Fortunately, the overall magnitude of this effect is rather small, and these errors will likely be unimportant in most scenarios.

The final test will be the displacement of a single Pb atom in a 216-atom supercell (see figure 4.10). The slave mode expansion is highly accurate even at displacements beyond 1.2 $\mathring{A}$. We believe these benchmarks demonstrate that our expansion is robust, and it should allow for simulations including both the effects of applied strain in addition to temperature. While some other approaches to the Taylor series expansion isolate the strain modes and treat them separately, the physics of strain is captured in our approach due to the fact that the anharmonic terms have decayed beyond the octahedron.

4.6 Minimal Model

Above we have demonstrated that our slave mode expansion accurately reproduces many key quantities. Nonetheless, it would be strongly desirable if we could somehow extract a *minimal* model of anharmonicity. It would be intuitive for the nearest-neighbor terms to be larger than the next nearest neighbor terms. When choosing the octahedral cluster, the nearest and next-nearest neighbor terms will be mixed. However, they can be separated. We will start by considering the dimer slave cluster of Pb-Te, where we will use the C_{4v} symmetry along the bond. Given that this case is three dimensional, the representation for the dimer will have six degrees of freedom, and projecting them onto the irreducible representations of the point group yields the following representation: $\Gamma = 2E \oplus 2A_1$. The representation for the modes which shift the dimer in the x, y, z directions can be chosen as one set of $E \oplus A_1$ and this must be removed leaving the following slave mode representation: $E \oplus A_1$. These modes can be explicitly constructed as follows:

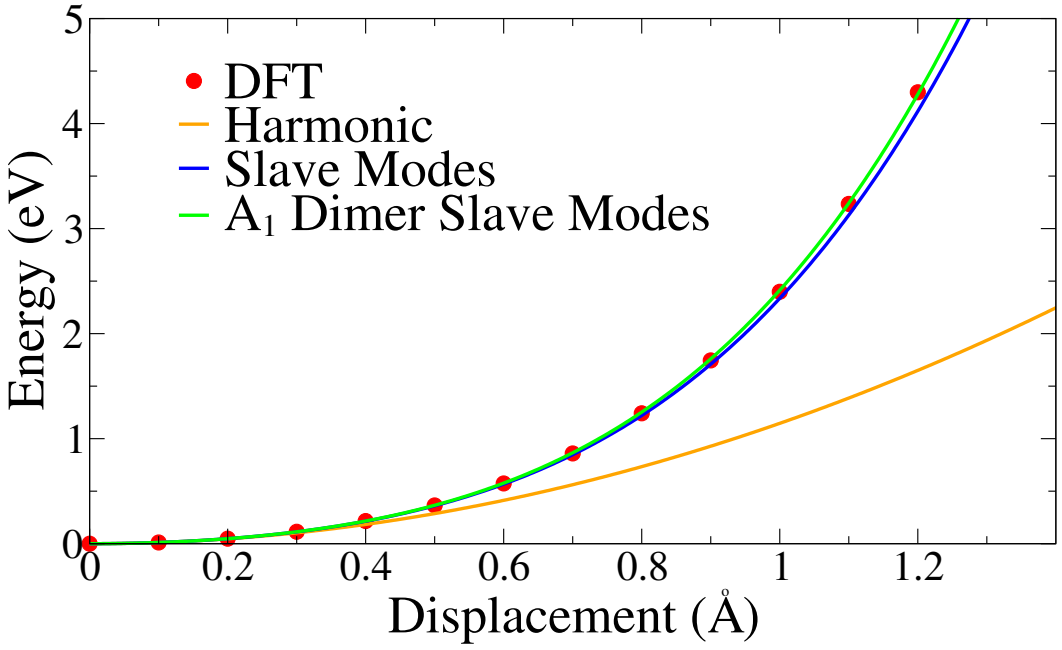

Figure 4.10: Energy as a function of displacing a single Pb atom in a 216 atom supercell along the $< -3, 1, 1 >$ direction. The green curve uses the minimal slave mode expansion which has only two expansion coefficients.

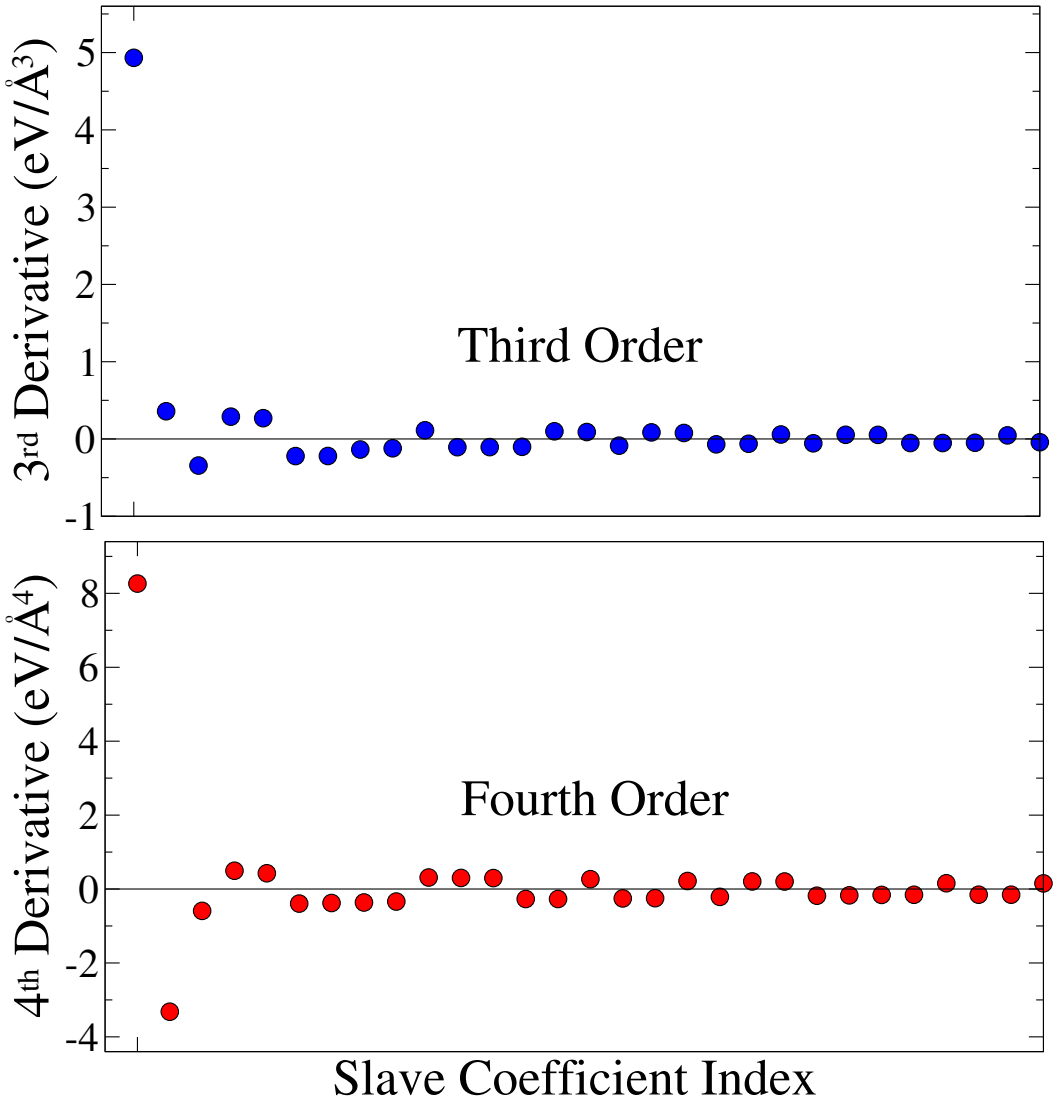

Figure 4.11: A plot of the transformed third and fourth order slave mode product coefficients Φ'. The values are ordered in decreasing magnitude. Only a fraction of the fourth order coefficients are shown.

$$\phi_{A_1} = \frac{1}{\sqrt{2}}(u_{Te,x} - u_{Pb,x}) \tag{4.1}$$
$$\phi_{E^{(1)}} = \frac{1}{\sqrt{2}}(u_{Te,y} - u_{Pb,y}) \;\; \phi_{E^{(2)}} = \frac{1}{\sqrt{2}}(u_{Te,z} - u_{Pb,z})$$

In this case we chose a cluster centered on a bond where the x-axis aligns with the 4-fold rotation axis. At third order there will be two terms: $\phi^3_{A_1}$ and $\phi_{A_1}\left(\phi^2_{E^{(1)}}+\phi^2_{E^{(2)}}\right)$. At fourth order there will be four terms:$\phi^4_{A_1}$ and $\phi^2_{A_1}\left(\phi^2_{E^{(1)}}+\phi^2_{E^{(2)}}\right)$ and $\phi^2_{E^{(1)}}\phi^2_{E^{(2)}}$ and $\phi^4_{E^{(1)}}+\phi^4_{E^{(2)}}$. The O_h symmetry center will then generate five more equivalent set of slave mode products for each case, one for each bond. We can add these terms to our original set of products in tables 5.1 and 5.2, but then we will need to remove two products at third order and four products at fourth order to regain an irreducible space. This is equivalent to performing a unitary transformation within the product space. After reconstructing the expansion coefficients for this new set of products, we then Gram-Schmidt orthogonalize all of the products starting from the dimer mode products. This physically motivated choice of phase convention in the product space achieves the goal of creating a minimal model in that there is now one dominant term at both third and fourth order (see figure 4.11). The dominant terms correspond to $\phi^3_{A_1}$ at third order and $\phi^4_{A_1}$ at fourth order. These two terms can be used to explicitly write a minimal model for the potential (we drop the A_1 index below):

$$
\begin{aligned}
&V = V_H + \\
&\Phi_3 \sum_{\mathbf{R}} (-\phi^3_{\mathbf{R}x_-} + \phi^3_{\mathbf{R}x_+} - \phi^3_{\mathbf{R}y_-} + \phi^3_{\mathbf{R}y_+} - \phi^3_{\mathbf{R}z_-} + \phi^3_{\mathbf{R}z_+}) + \\
&\Phi_4 \sum_{\mathbf{R}} (\phi^4_{\mathbf{R}x_-} + \phi^4_{\mathbf{R}x_+} + \phi^4_{\mathbf{R}y_-} + \phi^4_{\mathbf{R}y_+} + \phi^4_{\mathbf{R}z_-} + \phi^4_{\mathbf{R}z_+})
\end{aligned}
\tag{4.2}
$$

and:

$$
\begin{aligned}
\phi_{\mathbf{R}z_-} &= \tfrac{1}{\sqrt{2}}(u^{\mathbf{R}+\mathbf{a_1}}_{Te,z} - u^{\mathbf{R}}_{Pb,z}) \quad \phi_{\mathbf{R}z_+} = \tfrac{1}{\sqrt{2}}(u^{\mathbf{R}+\mathbf{a_2}+\mathbf{a_3}}_{Te,z} - u^{\mathbf{R}}_{Pb,z}) \\
\phi_{\mathbf{R}x_-} &= \tfrac{1}{\sqrt{2}}(u^{\mathbf{R}+\mathbf{a_2}}_{Te,x} - u^{\mathbf{R}}_{Pb,x}) \quad \phi_{\mathbf{R}x_+} = \tfrac{1}{\sqrt{2}}(u^{\mathbf{R}+\mathbf{a_1}+\mathbf{a_3}}_{Te,x} - u^{\mathbf{R}}_{Pb,x}) \\
\phi_{\mathbf{R}y_-} &= \tfrac{1}{\sqrt{2}}(u^{\mathbf{R}+\mathbf{a_3}}_{Te,y} - u^{\mathbf{R}}_{Pb,y}) \quad \phi_{\mathbf{R}y_+} = \tfrac{1}{\sqrt{2}}(u^{\mathbf{R}+\mathbf{a_1}+\mathbf{a_2}}_{Te,y} - u^{\mathbf{R}}_{Pb,y})
\end{aligned}
$$

Where V_H is the harmonic part of the potential, ϕ are the slave modes for the dimer, u are the atomic displacements, and $\mathbf{a_i}$ are the primitive lattice vectors of PbTe. There are six dimer slave modes per primitive unit cell, one corresponding to each Pb-Te octahedral bond, and these are simply a displacement difference between corresponding vectors of Pb and Te. The values for the expansion coefficients are found to be $\Phi_3 = 2.68eV/\mathring{A}^3$ and $\Phi_4 = 3.70eV/\mathring{A}^4$, respectively. The values in figure 4.11 are normalized in the space of monomials in order to have a meaningful relative comparison, whereas the preceding values are consistent with the prefactors in equation 4.2.

We can test the reliability of using only these two parameters by recomputing the optical modes under strain (see figure 4.9) and the energy of displacing a single atom

(see figure 4.10), displaying excellent agreement with the full expansion. Thereafter, this minimal model is then used to capture the anomalous temperature dependence of the phonon spectra in PbTeChen *et al.* (2014), which yields excellent result and is shown in Fig. 4.12.

There is one other term at fourth order which, though smaller, stands out among the other terms. This corresponds to $\phi^2_{A_1}\left(\phi^2_{E^{(1)}}+\phi^2_{E^{(2)}}\right)$ and has a coefficient of $-1.37eV/\mathring{A}^4$. We conclude this section by pointing out that this procedure for constructing a minimal model could be used in any scenario, though it is unclear if it will be as useful.

4.7 Conclusions

In conclusion, we have applied the slave mode expansion to generate the interatomic potential for PbTe. We used a finite difference approach to compute the slave mode coefficients, and accurately determined all 358 terms within fourth order and next nearest neighbor coupling. Examining the energy, stress, and phonons under lattice strain indicated that our expansion parameters are robust and that terms outside of the octahedron are relatively small. Furthermore, we have introduced an additional approach to perform a unitary transformation that allows us to accurately compress 56 cubic terms to one term and the 302 quartic terms to one term. This two parameter model of anharmonicity in PbTe has already been separately used to compute the temperature dependent phonon spectrum in the classical limit, resolving a major experimental anomalyChen *et al.* (2014). Our slave mode expansion should be broadly applicable to highly symmetric materials. While substantial resources have been dedicated to characterizing minimal models of electronic Hamiltonians, much less has been done in terms of characterizing anharmonic phonon interactions of relevant materials. Our approach should make this task substantially more tractable.

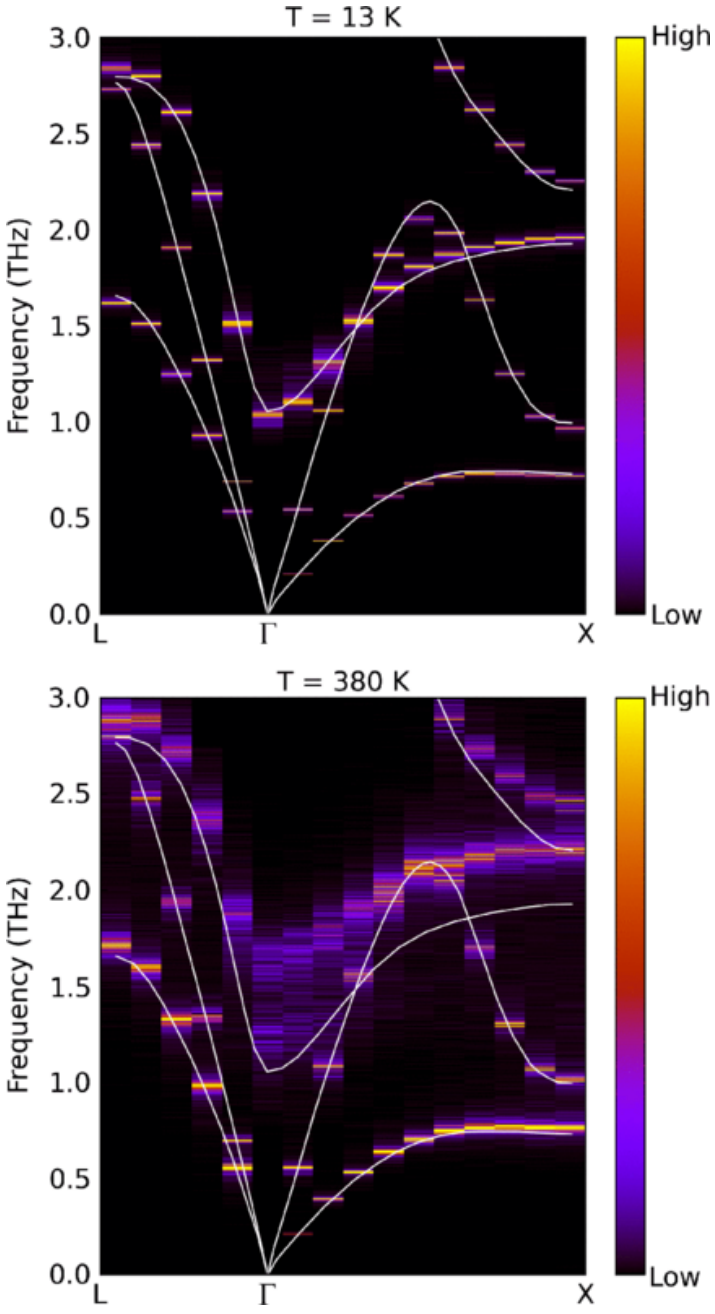

Figure 4.12: The classical vibrational spectra of PbTe along the high symmetry directions in the first Brillouin zone. The white lines show the 0 K phonon dispersions calculated with the finite displacement method by Zhang et al. Zhang *et al.* (2009) (from Chen *et al.* (2014))

Chapter 5

Application in Graphene

In this chapter, we will be applying the slave mode expansion to obtaining an ab-initio interatomic potential for graphene. The potential will be expanded up to 5th order to better capture the famous K1 mode instability in graphene, with interaction constrained within a hexagon. It is then assessed in the way that it predicts the energy and stress, as well as phonon dispersion; and it is found that the potential works well up to substantial strains in all cases. On the other hand, the phonon dispersion under strain predicted by the potentials up to various orders implies that the softening of K1 mode at K point is caused by its odd order terms.

5.1 Graphene and its K1 Mode Phonon Softening at K point

Graphene is a two dimensional material with honeycomb lattice structure with two atoms in one primitive cell. We will choose a primitive cell having vectors $a_1 = a/2(\sqrt{3}, 1, 0)$, $a_2 = a(0, 1, 0)$, $a_3 = c(0, 0, 1)$ (a = 2.45063 $\mathring{A}$ and c = 14 $\mathring{A}$ Isaacs and Marianetti (2014)), with one C atom at (0, 0, 0) and the other C atom at $(\frac{1}{3}, \frac{2}{3}, 0)$ (fractional coordinates). The point group symmetry of ideal single graphene layer is D_{6h} Kosti *et al.* (2009).

First-principles study on graphene reveals that its K1 mode phonon becomes soft under 0.151 equibiaxial strainMarianetti and Yevick (2010); its softening process is shown in Fig. 5.1, as indicated by the arrows. Experiments have been carried out to study this behavior, but the implied breaking strain far exceeds the theoretical results mentioned aboveLee *et al.* (2008). Since this mismatch is partly caused by the fact that experiments are conducted under finite temperature while the theoretical results are achieved under zero temperature, we would be generating an interatomic potential via slave mode expansion to facilitate finite-temperature theoretical studies.

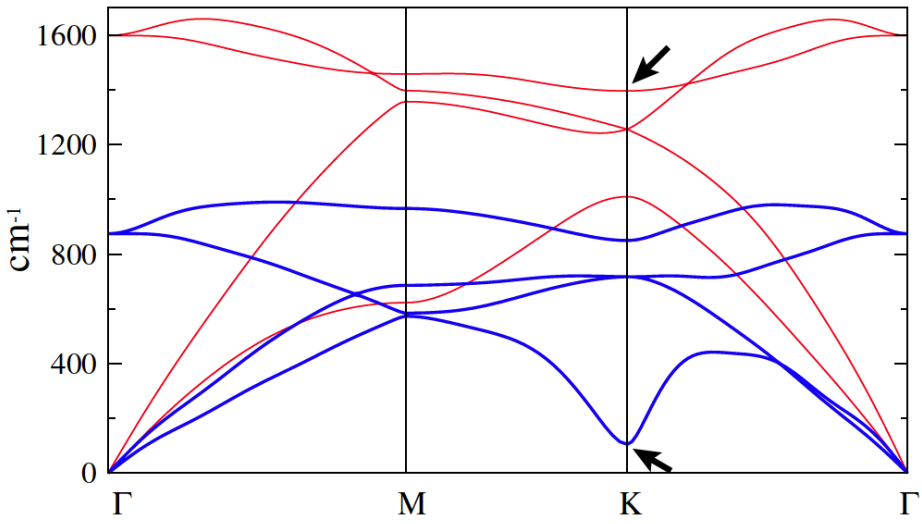

Figure 5.1: The in-plane phonons of graphene under equibiaxial strain. Thin red lines and thick blue lines correspond to $\epsilon_A = 0$ and $\epsilon_A = 0.205$, respectively. A black arrow is used to identify the K_1 mode. The k point labels Γ, M, K correspond to (0,0), (0.5, 0), (1/3, 1/3), respectively, in fractions of the reciprocal lattice vectors. (from paper Marianetti and Yevick (2010))

Our expansion would then be assessed by the comparison of the potential-predicted energy, stress and phonon dispersion under strain with first-principles results.

5.2 Group Theory Analysis

To construct the slave modes so that to expand the interatomic potential for graphene, one starts with the selection of atomic cluster(s). Instead of two triangles - one with center and the other without center, we decided to use the hexagonal atomic cluster since only one cluster type will be needed and it satisfies the D_{6h} point symmetry of the lattice. An illustration of it is in Fig. 5.2 with the atoms indexed.

As in the case of PbTe, the Cartesian coordinate system is used and the representation for the x, y and z displacements of the atoms within the hexagonal cluster could then be decomposed into modes that transform like the irreducible representations of

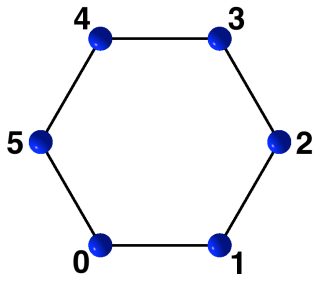

Figure 5.2: Hexgonal cluster with atoms indexed

D_{6h}[1]: $\Gamma = A_{1g} \oplus A_{2g} \oplus B_{2g} \oplus 2E_{2g} \oplus E_{1g} \oplus A_{2u} \oplus B_{1u} \oplus B_{2u} \oplus E_{2u} \oplus 2E_{1u}$. These modes are shown in Fig. 5.3. It could be observed that A_{2u} is a pure z shift mode. In addition, because two linearly independent combinations of the E_{1u}(it is two-dimensional and there are two) components are pure shifts, one set of E_{1u} can be chosen to be these shifts and the other will then be modes that are orthogonal to these shifts. The shift modes would thereafter be removed and the slave mode representation ends up to be $A_{1g} \oplus A_{2g} \oplus B_{2g} \oplus 2E_{2g} \oplus E_{1g} \oplus B_{1u} \oplus B_{2u} \oplus E_{2u} \oplus E_{1u}$. Fig. 5.3 also shows that in-plane modes and out-of-plane modes are completely decoupled – A_{2u}, B_{2g}, E_{1g} and E_{2u} are purely out-of-plane modes while the others $(A_{1g}, A_{2g}, 2E_{2g}, B_{1u}, B_{2u}, E_{1u})$ are purely in-plane modes. On the other hand, to derive these purely in-plane modes from the scratch, one could also repeat the whole process using the $2dD_{6h}$ symmetry and the representation of the x and y displacements of the atoms within a hexagonal cluster would be decomposed as $\Gamma = A_{1g} \oplus A_{2g} \oplus 2E_{2g} \oplus B_{1u} \oplus B_{2u} \oplus 2E_{1u}$. As above, only one set of E_{1u} would be kept after removing pure shift components and one achieves the same result.

Thereafter, a potential with symmetry imposed *apriori* could be expanded using the slave modes. However, for simplicity, we focus on a potential with just in-plane degrees of freedom – i.e. an expansion using the in-plane slave modes.

[1] Important notice for T_d and D_{6h} point group: when decomposing the representation, the components of a mode should be orthogonal to each other, otherwise, its character could be wrong.

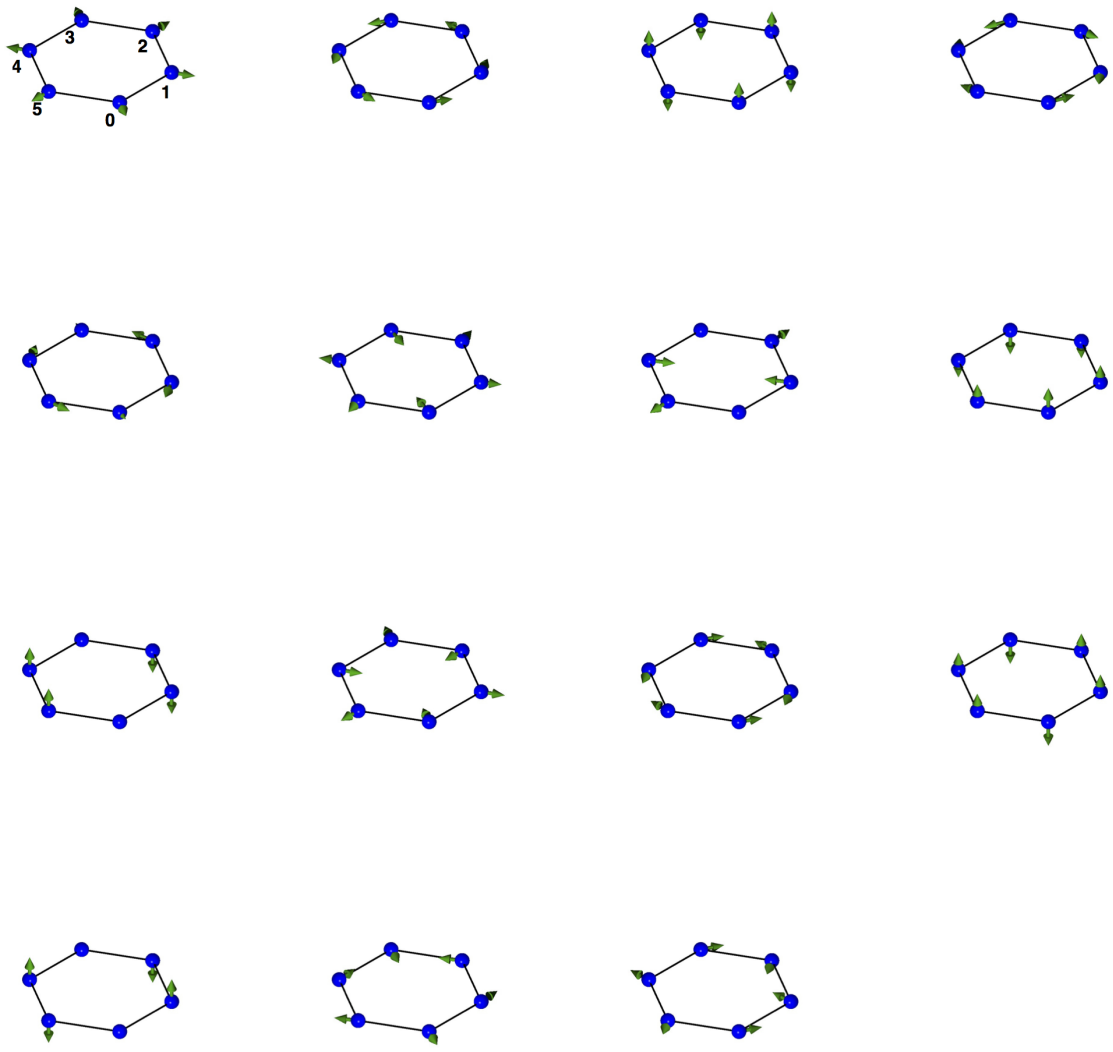

Figure 5.3: Slave modes within a hexagon transforming as the irreducible representations of the point group. A_{2u} and one of E_{1u} modes which shift the hexagon have been removed. Reading from left to right and top to bottom, the modes are $A_{1g}, A_{2g}, B_{2g}, 2E_{2g}, E_{1g}, B_{1u}, E_{2u}$and E_{1u}

5.3 Slave Mode Expansion for Graphene

As in the PbTe case, we will assume that the harmonic terms have been computed using traditional approaches for computing phonons from first-principles, such as density functional perturbation theoryBaroni *et al.* (2001) or finite displacement supercell approachesAlfe (2009); Kunc and Martin (1982). Though it is therefore not necessary to form the 2nd order slave mode expansion, it is worth checking as they could be conveniently derived by hand and there are just 7 of them.

In this thesis, the third, fourth and fifth order slave mode expansion terms will be derived for the potential of graphene. In details, third and fourth order ones are achieved via slave modes within a hexagonal cluster, and fifth order ones are accomplished using slave modes within a dimer (e.g. the two atoms forming bond 01 in Fig. 5.2)– we call them dimer modes.

5.3.1 Third and Fourth Order

To derive the third and fourth order terms that transform like identities, one could either select a linearly independent subset after forming the product representation or try the symmetric products. We use the former approach and end up with 20 unique identities at third order and 70 unique ones at fourth order. Constructing the $\mathcal{V}$ matrice does not further reduce the number. The products, together with phase and corresponding coefficients, are listed in Table 5.1 and Table 5.2; the phase convention is defined in Chapter 3 and how the coefficients are computed will be presented in Sec. 5.4. On the other hand, the CG coefficients we derived at the same time for all the terms are provided in Appendix E so that the terms could be conveniently reproduced.

5.3.2 Fifth Order

Then we derived the fifth order terms. However, computing all fifth order terms using slave modes within a hexagon is a little bit unrealistic. Therefore, we decided to derive them using dimer modes.

As in the square lattice case, there is one A_1 mode and one A_2 mode within a dimer. So there would be three identities – $\Phi^5_{A_1}$, $\Phi^3_{A_1}\Phi^2_{A_2}$, and $\Phi_{A_1}\Phi^4_{A_2}$ – on each bond of the hexagon at 5th order. The $\Phi^d_{A_1}$s and $\Phi^d_{A_2}$s (d superscript indexes dimer) within each of the dimers are listed in Table 5.3. Next, to preserve the $2dD_{6h}$ point symmetry of graphene, one needs to sum them up as they are mapped into each other

product	Phase	Coefficient
$A_{1g} \otimes B_{1u} \otimes B_{1u}$	1	-0.257
$A_{2g} \otimes B_{1u} \otimes B_{2u}$	1	0.155
$2E_{2g} \otimes 2E_{2g} \otimes 2E_{2g}$	11, 16, 32, 1	-106.838, -104.54, -2.63, -40.04
$2E_{2g} \otimes B_{1u} \otimes E_{1u}$	3, 4	1.002, -14.845
$A_{1g} \otimes 2E_{2g} \otimes 2E_{2g}$	4, 1, 2	-5.452, -5.053, 24.927
$A_{2g} \otimes 2E_{2g} \otimes 2E_{2g}$	12	-5.186
$A_{1g} \otimes A_{1g} \otimes A_{1g}$	1	-0.364
$A_{1g} \otimes E_{1u} \otimes E_{1u}$	4	-3.077
$2E_{2g} \otimes E_{1u} \otimes E_{1u}$	13, 8	-9.358, -7.22
$2E_{2g} \otimes B_{2u} \otimes E_{1u}$	6, 5	0.268, 58.317
$A_{1g} \otimes A_{2g} \otimes A_{2g}$	1	0.103
$A_{1g} \otimes B_{2u} \otimes B_{2u}$	1	-2.338

Table 5.1: Nonzero third order products and the corresponding term coefficients. The second column indexes the basis of the product space which gives the identity after projection operator is applied.

by the symmetry operations. Thus, the 5th order terms will be $\Psi_1 = \sum_d (\Phi^d_{A_1})^5$, $\Psi_2 = \sum_d (\Phi^d_{A_1})^3 (\Phi^d_{A_2})^2$ and $\Psi_3 = \sum_d \Phi^d_{A_1} (\Phi^d_{A_2})^4$.

5.4 Computing Expansion Coefficients for Graphene

Having determined the slave mode expansion up to fifth order and within a hexagon, the slave mode coefficients could now be computed. As described in Chapter 3, the monomial coefficients will be computed first and then mapped back to achieve the slave mode coefficients. The mapping matrices are preconditioned so that to reduce the propagation of noises from DFT runs to the slave mode coefficients; and this leads to the selection of a set of monomials. In our case of graphene, we selected and computed 22 monomial coefficients at third order and 82 at fourth order; they are listed in Table 5.4 and 5.5.

product	**Phase**	**Coefficient**
$2E_{2g} \otimes 2E_{2g} \otimes B_{2u} \otimes B_{2u}$	12, 3, 4	10.675, -0.494, -4.672
$A_{1g} \otimes A_{1g} \otimes A_{1g} \otimes A_{1g}$	1	6.949
$A_{2g} \otimes A_{2g} \otimes 2E_{2g} \otimes 2E_{2g}$	6, 7, 11	-1.225, -20.575, -403.718
$A_{1g} \otimes 2E_{2g} \otimes 2E_{2g} \otimes 2E_{2g}$	48, 2, 11, 28	11.538, -4.903, 0.257, 4.989
$A_{1g} \otimes A_{1g} \otimes A_{2g} \otimes A_{2g}$	1	-49.49
$2E_{2g} \otimes 2E_{2g} \otimes B_{1u} \otimes E_{1u}$	16, 5, 7	13.774, -1.062, -1.721
$2E_{2g} \otimes 2E_{2g} \otimes E_{1u} \otimes E_{1u}$	24, 10, 64, 28, 16, 42	13.681, -4.896, 6.596, -384.977, -26.123, -0.844
$A_{1g} \otimes 2E_{2g} \otimes B_{2u} \otimes E_{1u}$	7, 6	52.049, -0.566
$B_{1u} \otimes B_{1u} \otimes E_{1u} \otimes E_{1u}$	2	28.558
$A_{1g} \otimes A_{1g} \otimes B_{1u} \otimes B_{1u}$	1	0.207
$B_{1u} \otimes B_{1u} \otimes B_{1u} \otimes B_{1u}$	1	-0.147
$2E_{2g} \otimes 2E_{2g} \otimes B_{1u} \otimes B_{1u}$	8, 3, 1	-131.096, -35.311, -0.089
$A_{2g} \otimes A_{2g} \otimes B_{1u} \otimes B_{1u}$	1	2.404
$A_{2g} \otimes A_{2g} \otimes E_{1u} \otimes E_{1u}$	1	-0.851
$A_{1g} \otimes 2E_{2g} \otimes E_{1u} \otimes E_{1u}$	4, 2	1.133, -5.452
$2E_{2g} \otimes 2E_{2g} \otimes B_{2u} \otimes E_{1u}$	16, 11, 4	-51.4, -46.789, 14.237
$A_{2g} \otimes 2E_{2g} \otimes E_{1u} \otimes E_{1u}$	4, 12	-0.308, -126.366
$E_{1u} \otimes E_{1u} \otimes E_{1u} \otimes E_{1u}$	2	-0.361
$A_{2g} \otimes 2E_{2g} \otimes 2E_{2g} \otimes 2E_{2g}$	27, 3, 2, 24	-17.453, 4.85, 40.346, 3.381
$A_{1g} \otimes A_{1g} \otimes E_{1u} \otimes E_{1u}$	2	11.717
$A_{1g} \otimes A_{1g} \otimes 2E_{2g} \otimes 2E_{2g}$	12, 16, 6	-23.73, -100.103, -1.279
$B_{1u} \otimes E_{1u} \otimes E_{1u} \otimes E_{1u}$	1	-36.3
$B_{2u} \otimes B_{2u} \otimes E_{1u} \otimes E_{1u}$	4	0.094
$B_{1u} \otimes B_{1u} \otimes B_{2u} \otimes B_{2u}$	1	-8.701
$A_{2g} \otimes 2E_{2g} \otimes B_{1u} \otimes E_{1u}$	2, 5	10.428, -2.073
$2E_{2g} \otimes 2E_{2g} \otimes B_{1u} \otimes B_{2u}$	8	6.783
$A_{1g} \otimes A_{2g} \otimes 2E_{2g} \otimes 2E_{2g}$	11	112.172
$A_{1g} \otimes A_{1g} \otimes B_{2u} \otimes B_{2u}$	1	47.572
$A_{2g} \otimes A_{2g} \otimes B_{2u} \otimes B_{2u}$	1	-3.272
$A_{2g} \otimes A_{2g} \otimes A_{2g} \otimes A_{2g}$	1	2.897
$A_{2g} \otimes 2E_{2g} \otimes B_{2u} \otimes E_{1u}$	5, 2	-0.716, 2.898
$B_{2u} \otimes E_{1u} \otimes E_{1u} \otimes E_{1u}$	1	1.44
$B_{2u} \otimes B_{2u} \otimes B_{2u} \otimes B_{2u}$	1	0.143
$A_{1g} \otimes 2E_{2g} \otimes B_{1u} \otimes E_{1u}$	2, 4	-0.015, 7.929
$2E_{2g} \otimes 2E_{2g} \otimes 2E_{2g} \otimes 2E_{2g}$	64, 3, 1, 48, 176, 8	1.076, 54.983, 128.889, -480.892, -314.137, 95.792
$A_{1g} \otimes A_{2g} \otimes B_{1u} \otimes B_{2u}$	1	137.622

Table 5.2: Nonzero fourth order products and the corresponding term coefficients. The second column indexes the basis of the product space which gives the identity after projection operator is applied.

Dimer	Φ_{A_1}	Φ_{A_2}
dimer 01	$\Phi^{01}_{A_1} = x_1 - x_0$	$\Phi^{01}_{A_2} = y_1 - y_0$
dimer 12	$\Phi^{12}_{A_1} = -\frac{1}{2}x_1 + \frac{1}{2}x_2 - \frac{\sqrt{3}}{2}y_1 + \frac{\sqrt{3}}{2}y_2$	$\Phi^{12}_{A_2} = \frac{\sqrt{3}}{2}x_1 - \frac{\sqrt{3}}{2}x_2 - \frac{1}{2}y_1 + \frac{1}{2}y_2$
dimer 23	$\Phi^{23}_{A_1} = \frac{1}{2}x_2 - \frac{1}{2}x_3 - \frac{\sqrt{3}}{2}y_2 + \frac{\sqrt{3}}{2}y_3$	$\Phi^{23}_{A_2} = \frac{\sqrt{3}}{2}x_2 - \frac{\sqrt{3}}{2}x_3 + \frac{1}{2}y_2 - \frac{1}{2}y_3$
dimer 34	$\Phi^{34}_{A_1} = x_3 - x_4$	$\Phi^{34}_{A_2} = y_3 - y_4$
dimer 45	$\Phi^{45}_{A_1} = \frac{1}{2}x_4 - \frac{1}{2}x_5 + \frac{\sqrt{3}}{2}y_4 - \frac{\sqrt{3}}{2}y_5$	$\Phi^{45}_{A_2} = -\frac{\sqrt{3}}{2}x_4 + \frac{\sqrt{3}}{2}x_5 + \frac{1}{2}y_4 - \frac{1}{2}y_5$
dimer 50	$\Phi^{50}_{A_1} = \frac{1}{2}x_0 - \frac{1}{2}x_5 - \frac{\sqrt{3}}{2}y_0 + \frac{\sqrt{3}}{2}y_5$	$\Phi^{50}_{A_2} = \frac{\sqrt{3}}{2}x_0 - \frac{\sqrt{3}}{2}x_5 + \frac{1}{2}y_0 - \frac{1}{2}y_5$

Table 5.3: Table recording the A_1 and B_1 modes on the bond dimers within a hexagon; dimer xy refers to dimer formed by atom x and atom y as indexed in Fig. 5.2

5.4.1 DFT Runs and Finite Difference

As outlined in Chapter 3, the monomial coefficients are computed with finite difference. Given that the forces are known from the Hellman-Feynman TheoremMartin (2008), the first derivatives will all be known for a given DFT computation. Using the central finite difference, one could then approximate higher order derivatives according to Eqn. 3.4.

VASP setup

The forces are computed within the framework of Density Functional Theory which is carried out with the Projector Augmented-wave potentials (PAW)Blöchl (1994); Kresse and Joubert (1999b) in the Vienna ab initio simulation package(VASP)Kresse and Hafner (1993, 1994); Kresse and Furthmuller (1996a,b); Kresse and Joubert (1999a). Gamma centered k-meshes are applied and a $6 \times 6 \times 1$ mesh is used for all the supercell sizes from 128-atom one to 162-atom one. Charge self-consistency is performed until the energy is converged to within 10^{-6} eV, and a plane wave cutoff of $600eV$ was used depending on the particular computation. Spin-orbit coupling was not utilized.

Optimal Δ for Finite Difference

One should be careful when approximating the derivative using Finite Difference, i.e. choosing the optimal Δ. As discussed in Chapter 3, the approximation error in central finite difference is quadratic, which indicates that if Δ is too large, the error tail hides the true value of the derivative. On the other hand, if Δ is too small, the magnified noises of the data hides it. Therefore, the optimal Δ is usually located somewhere in between.

The aforementioned finite difference vs. Δ pattern could be clearly observed in Fig. 5.4, with the upper one displaying the approximation for $\frac{\partial^3 E}{\partial x_1^3}$ and the lower one displaying that for $\frac{\partial^4 E}{\partial x_0^4}$. The finite difference values computed from the DFT data are plotted as red dots while the dots with larger Δs are fitted into a quadratic blue curve which verifies the order of the approximation error. It could then be figured out from these plots that the optimal Δs for the two cases should then be located somewhere around $0.03\mathring{A}$. This pattern also exists in the other third order finite difference approximations. However, there are cases, i.e. 4th and 5th order finite difference approximations – especially those with smaller magnitudes, that do not share such a clear pattern so that a universal value for the optimal Δ could not be predetermined; and one has to visualize the finite difference for a range of Δs and pick the optimal one manually thereafter. Examples are given in Fig. 5.5 and Fig. 5.6.

Optimal Supercell Size for Finite Difference

Aside from choosing the optimal Δ for finite difference, one must also test for its convergence with respect to supercell size – to be sure that images are not interacting with one another. In order to illustrate this, we plot some finite differences vs. Δ in Fig. 5.7 and Fig. 5.8 and compare the results from different supercell sizes that are indicated by different colors. The plots demonstrate that the changes in the approximations are diminishing with increasing cell size. We finally decided to use 162-atom supercells for 3rd order finite difference and 128-atom supercells for 4th order finite difference.

5.4.2 Slave Mode Expansion Coefficients

As mentioned in the beginning, we have computed 22 monomial coefficients at third order, 82 at fourth order and 4 at fifth order, as listed in Table 5.4 and 5.5. These numbers exceed the numbers of slave mode coefficients, and therefore we have sets of overdetermined equations that uniquely determine the slave mode coefficients. Singular value decomposition is then used to find the optimum solution in terms of least squares and the final solutions for third and fourth order terms are plotted in Fig. 5.9. On the other hand, the values of each slave mode coefficient have already been listed in Tables 5.1 and 5.2.

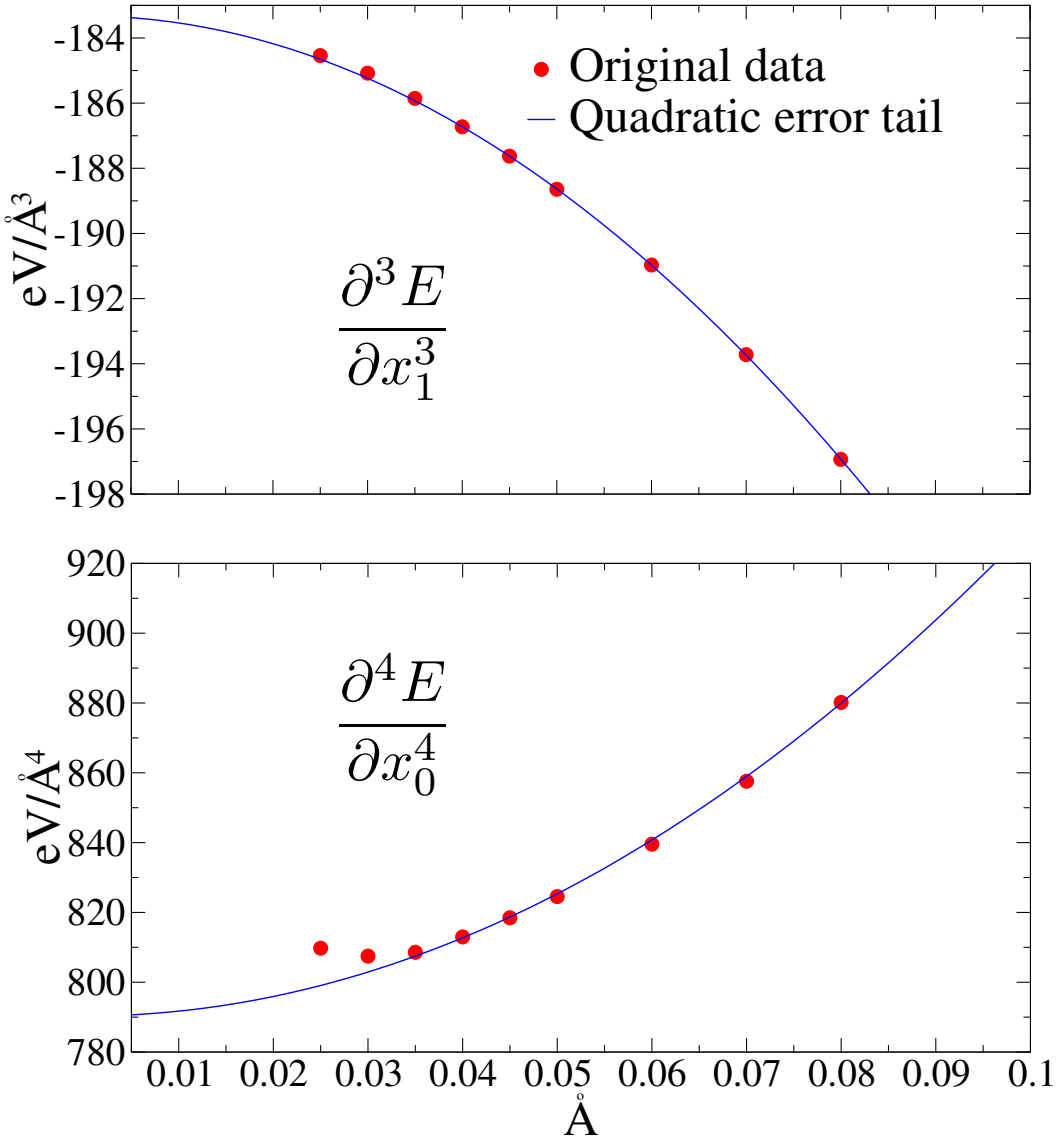

Figure 5.4: Finite difference approximation for $\frac{\partial^3 E}{\partial x_1^3}$ (upper) and $\frac{\partial^4 E}{\partial x_0^4}$ (lower) and vs. Δ.

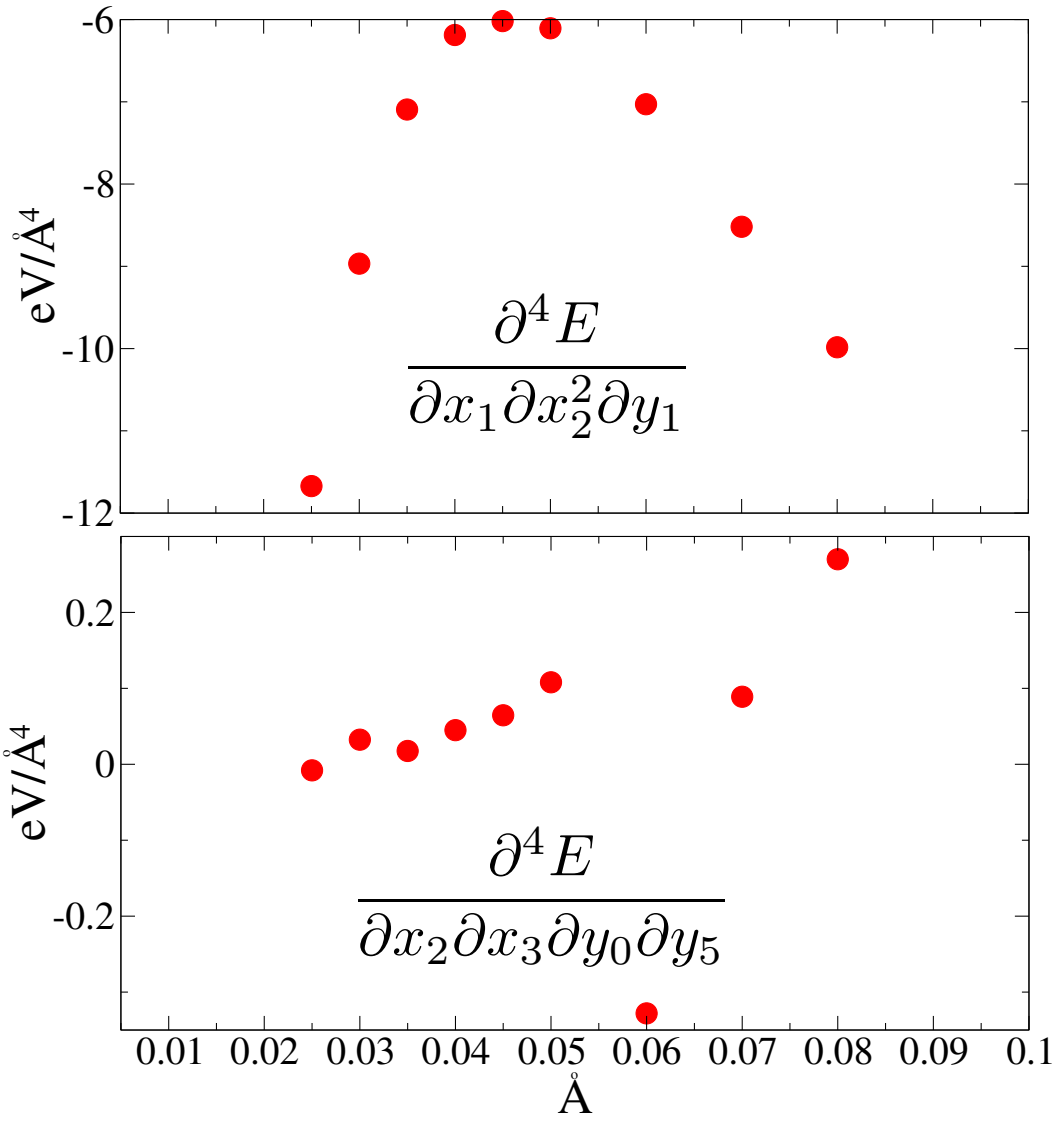

Figure 5.5: Finite difference approximation for $\frac{\partial^4 E}{\partial x_1 \partial x_2^2 \partial y_1}$ and $\frac{\partial^4 E}{\partial x_2 \partial x_3 \partial y_0 \partial y_5}$ vs. Δ

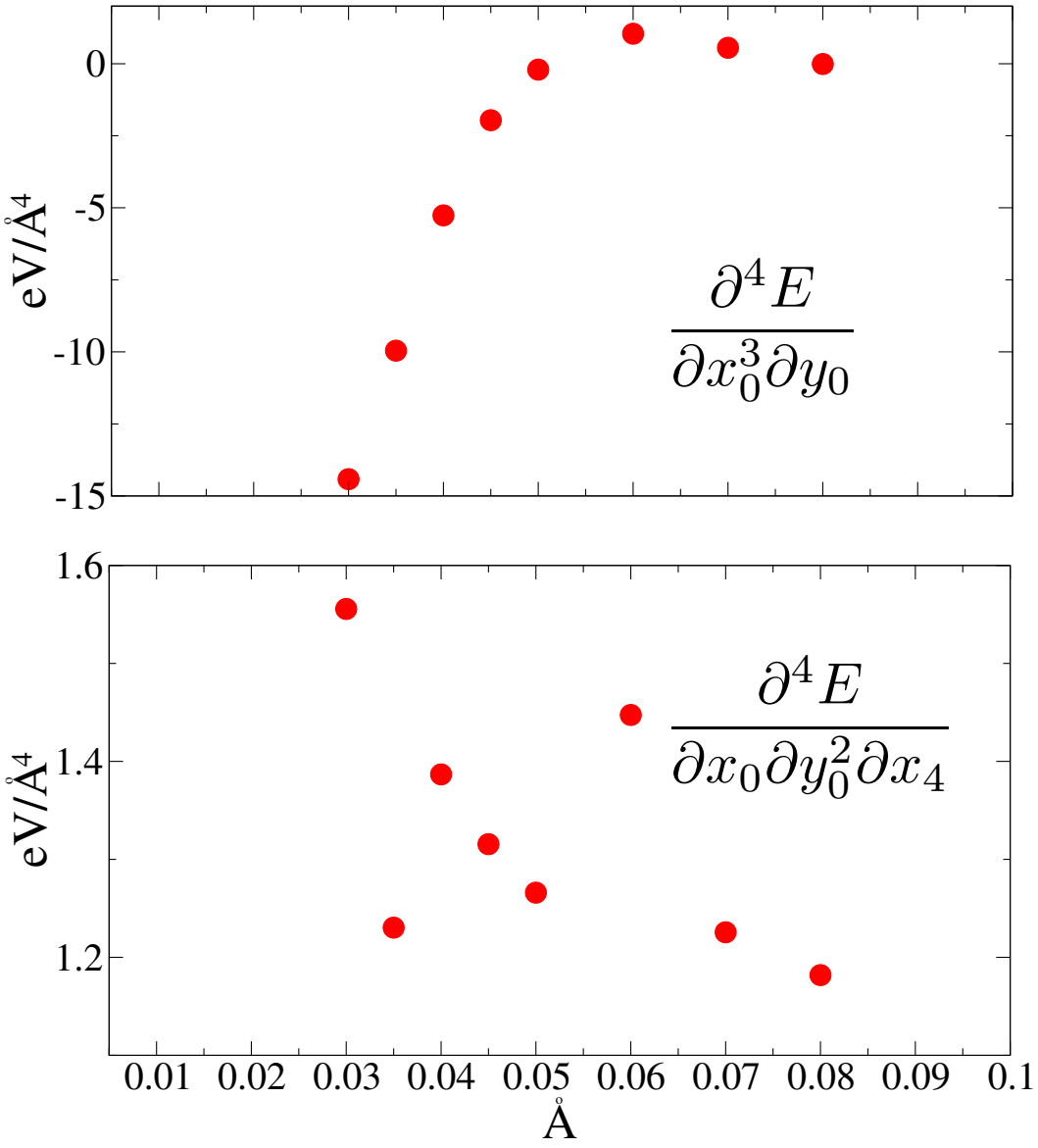

Figure 5.6: Finite difference approximation for $\frac{\partial^4 E}{\partial x_0^3 \partial y_0}$ and $\frac{\partial^4 E}{\partial x_0 \partial y_0^2 \partial x_4}$ vs. Δ

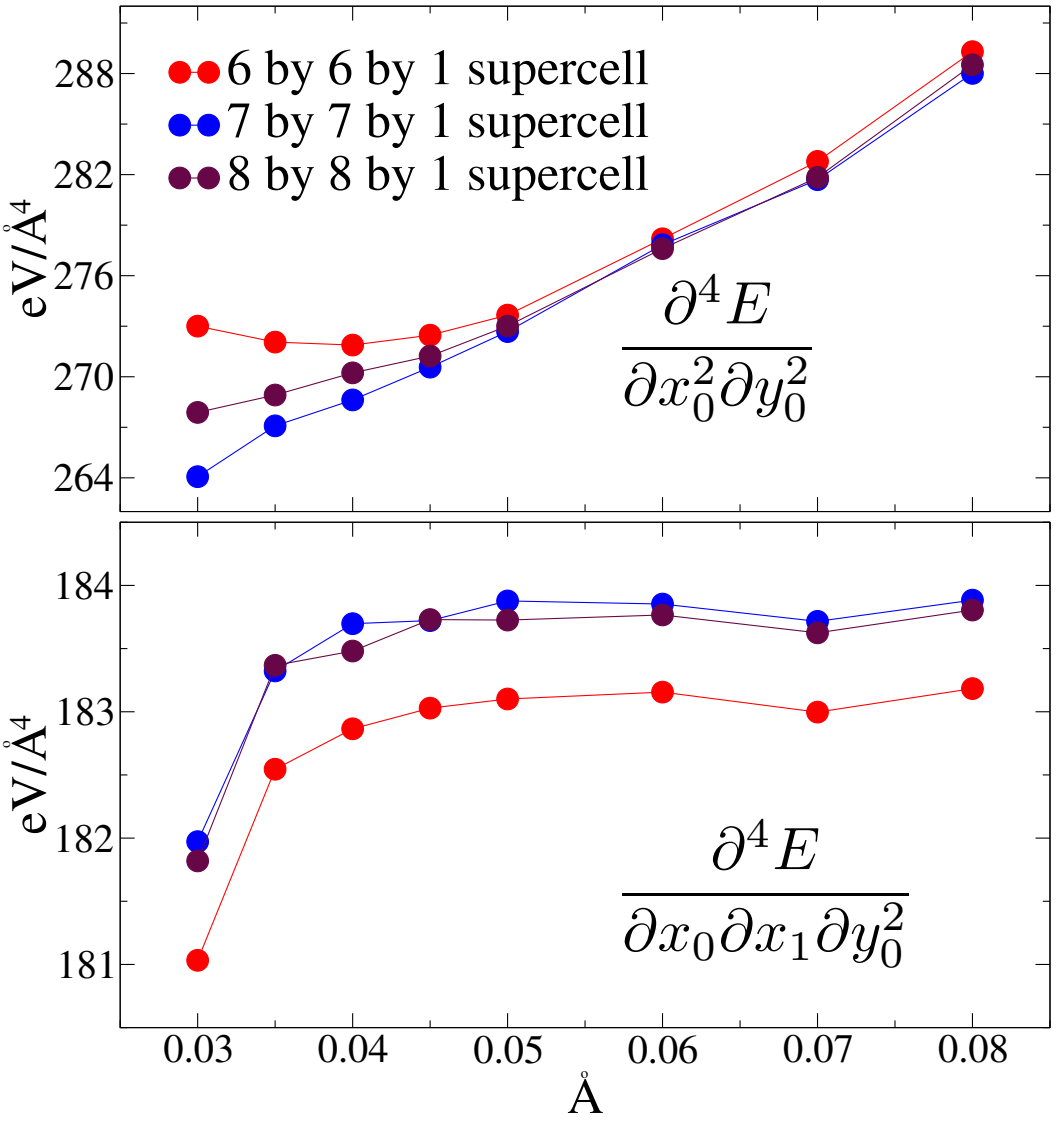

Figure 5.7: Finite difference approximation for $\frac{\partial^4 E}{\partial x_0^2 \partial y_0^2}$ and $\frac{\partial^4 E}{\partial x_0 \partial x_1 \partial y_0^2}$ vs. Δ. Different colors stand for different supercell size: red – 72-atom, blue – 98-atom and magneta – 128-atom

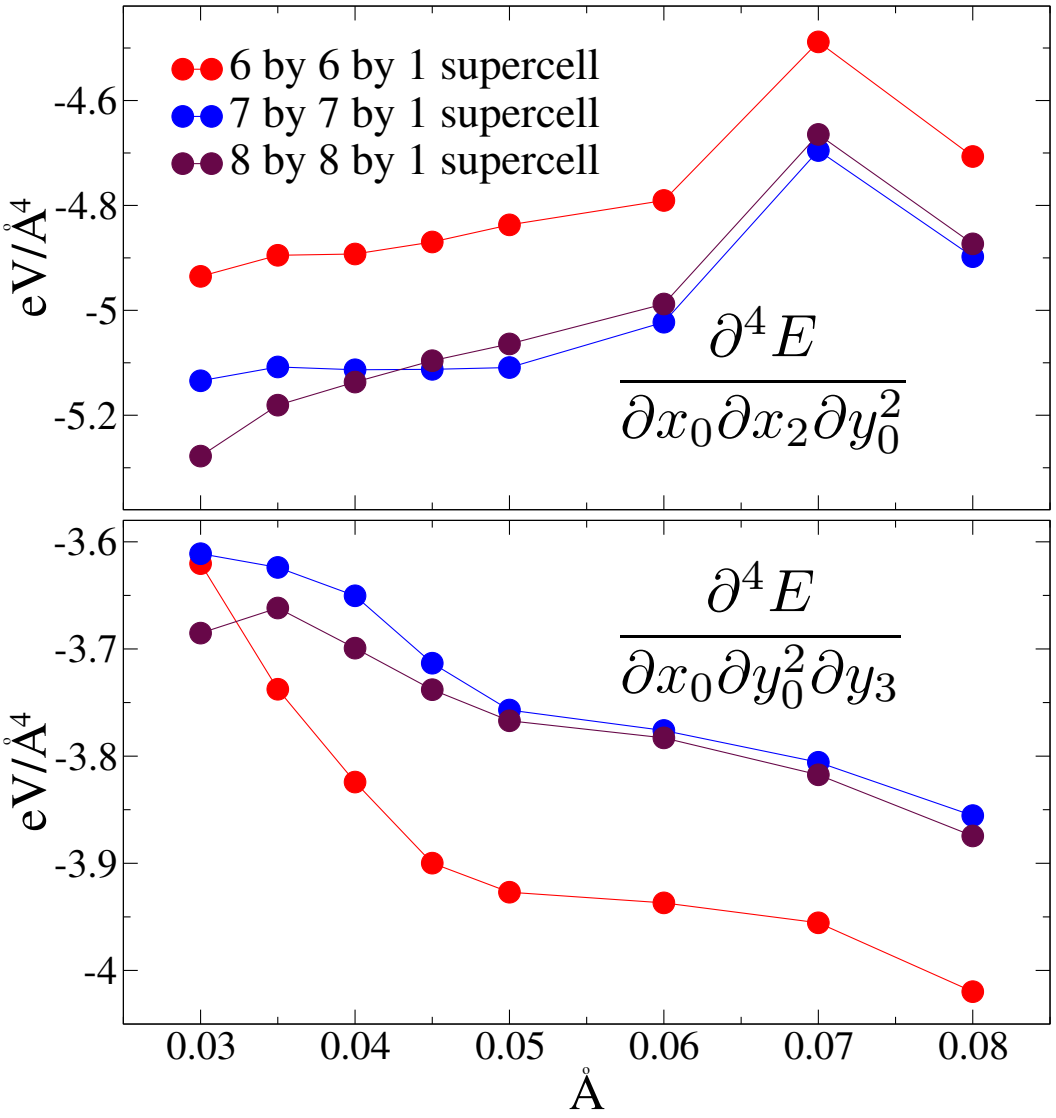

Figure 5.8: Finite difference approximation for $\frac{\partial^4 E}{\partial x_0 \partial x_2 \partial y_0^2}$ and $\frac{\partial^4 E}{\partial x_0 \partial y_0^2 \partial y_3}$ vs. Δ. Different colors stand for different supercell size: red – 72-atom, blue – 98-atom and magneta – 128-atom

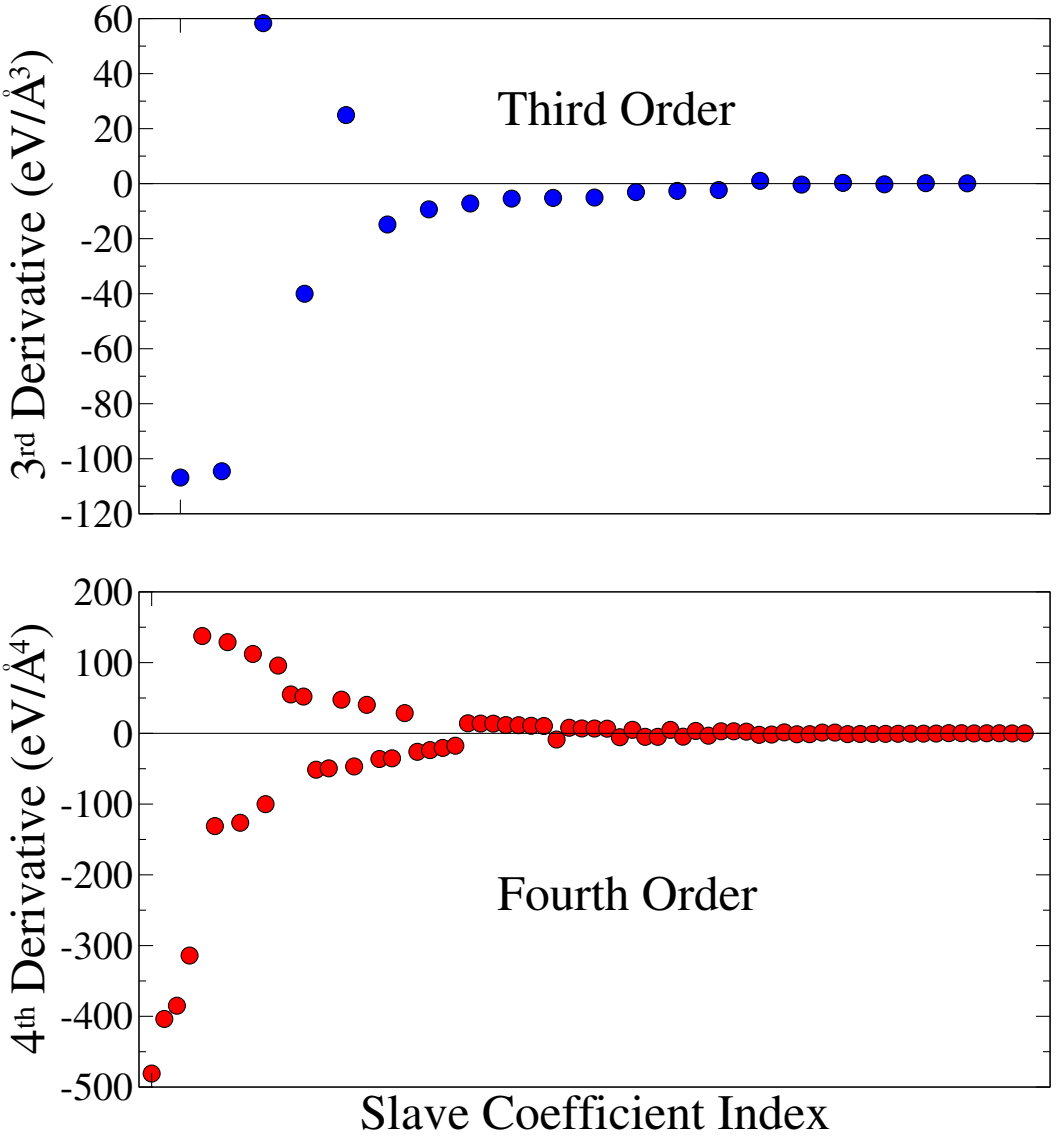

Figure 5.9: The 3rd order and 4th order coefficients for graphene, from the ones with the largest magnitude to those with the lowest magnitude

monomial	coefficient	monomial	coefficient
x_3^3	-30.982	$x_1^2x_2$	-5.911
$x_4y_0^2$	-0.332	$y_0y_3^2$	1.233
$x_1^2y_3$	1.058	$x_2^2y_3$	-21.534
$y_0^2y_3$	-1.237	$x_1^2y_4$	0.696
$y_0^2y_4$	-5.42	$x_0x_1x_4$	-1.42
$x_0x_1y_4$	-1.54	$x_0x_2y_4$	-0.451
$x_0y_2y_3$	0.6625	$x_0y_2y_4$	0.8836
$x_1x_3y_3$	-2.337	$x_1y_1y_4$	0.856
$x_2x_4y_3$	1.6275	$x_2y_0y_1$	0.897
$x_3y_0y_2$	-0.1097	$x_3y_2y_3$	-85.43875
$y_0y_1y_2$	-0.5564	$y_1y_3y_4$	-1.4847

Table 5.4: Third order monomial coefficients computed via Finite Difference.

5.5 Assessing the Expansion

Having computed the slave mode expansion coefficients up to fourth order and dimer term coefficients at fifth order and within a hexagon, we now evaluate the overall reliability of our expansion. The major point of concern in the method we have employed to compute the slave mode coefficients is whether or not the slave mode expansion is sufficiently converged within the hexagon or if non-negligible terms beyond

monomial	coefficient	monomial	coefficient	monomial	coefficient	monomial	coefficient
x_0^4	33.9795	$x_3y_0^3$	-1.207	$x_0^3y_3$	-0.5037	$x_0^2x_4^2$	0.379
$x_0^2y_4^2$	-3.774	$x_1^2x_2^2$	-33.468	$x_2^2y_3^2$	53.289	$x_3^2x_4^2$	271.759
$y_0^2y_4^2$	1.24	$x_0x_1x_2^2$	3.893	$x_0x_1^2x_2$	-10.328	$x_0x_2y_0^2$	-2.568
$x_0x_1^2x_3$	0.716	$x_0x_3y_0^2$	-0.632	$x_0x_3y_4^2$	0.519	$x_0x_4y_4^2$	0.694
$x_0x_4^2y_0$	1.608	$x_0y_0^2y_2$	0.308	$x_0x_2^2y_3$	0.065	$x_0x_1^2y_4$	-0.023
$x_0x_3^2y_4$	-0.821	$x_0y_0^2y_4$	1.062	$x_1x_3y_0^2$	-1.479	$x_1x_4y_4^2$	-0.602
$x_1x_2^2y_0$	0.090	$x_1x_4^2y_0$	-1.374	$x_1y_0y_2^2$	0.0335	$x_1y_0y_4^2$	0.537
$x_1x_3^2y_3$	1.226	$x_1x_2^2y_4$	-0.0926	$x_1x_4^2y_4$	-0.3465	$x_0^2x_2y_0$	-0.203
$x_2x_4^2y_0$	0.25	$x_2y_0y_1^2$	-0.223	$x_3y_0^2y_1$	-0.057	$x_2^2x_3y_2$	-3.703
$x_3y_2y_4^2$	0.324	$x_4y_0y_3^2$	-0.206	$x_4y_0^2y_1$	0.4565	$x_4y_1y_3^2$	0.853
$x_0^2x_4y_2$	0.462	$x_3^2x_4y_2$	-1.3955	$x_4y_2y_3^2$	0.1097	$x_0^2x_4y_3$	-0.492
$x_2^2x_4y_3$	-0.526	$x_4y_2^2y_3$	-1.859	$x_0^2x_4y_4$	-1.914	$x_4y_0^2y_4$	1.115
$x_2^2y_0y_1$	3.257	$x_0^2y_0y_2$	-3.087	$x_2^2y_0y_2$	-0.885	$y_0y_2y_4^2$	-0.426
$x_2^2y_0y_3$	0.319	$x_3^2y_0y_3$	-1.6525	$x_0^2y_1y_3$	1.535	$y_0^2y_1y_3$	-1.816
$y_1y_2^2y_3$	-10.5995	$x_3^2y_1y_4$	-0.883	$y_0^2y_1y_4$	1.527	$x_0^2y_2y_4$	0.271
$x_2^2y_2y_4$	-0.922	$x_0x_3x_4y_3$	-0.121	$x_0x_4y_0y_4$	-7.871	$x_1x_2x_3y_3$	-1.9825
$x_1x_2y_1y_2$	231.303	$x_1x_2y_2y_3$	-8.995	$x_1x_3x_4y_3$	0.193	$x_1x_4y_0y_4$	2.968
$x_1x_4y_3y_4$	-2.443	$x_1y_0y_1y_4$	-0.9	$x_1y_1y_2y_3$	0.201	$x_2x_3x_4y_3$	0.939
$x_2x_3y_0y_1$	0.234	$x_2x_3y_0y_2$	1.2	$x_2x_3y_0y_4$	0.0215	$x_2x_3y_2y_4$	-1.988
$x_2x_4y_0y_4$	0.529	$x_2x_4y_1y_2$	0.109	$x_2y_2y_3y_4$	-2.913	$x_3y_0y_2y_3$	-1.627
$x_4y_0y_1y_4$	-0.505	$x_4y_2y_3y_4$	0.019				

Table 5.5: Fourth order monomial coefficients computed via Finite Difference.

the hexagon are present. A potent test to address this issue is to use the slave mode expansion to compute energy, stress, and phonons as a function of lattice strain. It should be emphasized that our slave mode expansion is performed in the absence of any strain, but if our cluster is sufficiently large the expansion will be able to be used to compute the energetics under strain. Given that strain will amplify the coupling to long range interactions, and that it is straightforward to compute the answer to these tests using DFT, this serves as an ideal testbed for any type of Taylor series expansion in terms of atomic displacements.

5.5.1 Energy and Stress under Strain

The first test is to compute the energy and the stress as a function of strain (see figure 5.10). As shown, there is remarkable agreement in both energy and stress under strains as high as 20%. This favorable agreement suggests that longer range terms are not substantial.

5.5.2 Phonon Dispersion under Strain

A more stringent test is to compute the phonons as a function of strain and one could compare the phonon dispersions predicted by potentials up to different orders. Here we are going to try three types of strain – equibiaxial strain, strain along "Armchair" direction and strain along "Zigzag" direction.

Equibiaxial Strain

The first type of strain applied is an equibiaxial strain. From Fig. 5.11, one could observe that the phonon dispersion has a large change under a 0.05 strain from the upper plot and the potential up to 4th and 5th order exactly reproduced that change as seen from the lower plot. In addition, when it goes to a 0.1 strain in Fig. 5.12, the phonon dispersion has a even larger change and the 5th order potential starts to outperform the 4th order one by better replicating the lower branch of the upper two – which is also our motivation in deriving the 5th order terms. Though at this point the potential missed the physics of the softening of K_1 mode phonon at K mode, which might be caused by the possibility that the coupling could be longer-ranged than a hexagon, the 5th order terms take the K_1 mode at K point down closer to something soft when strain is increased to 0.15.

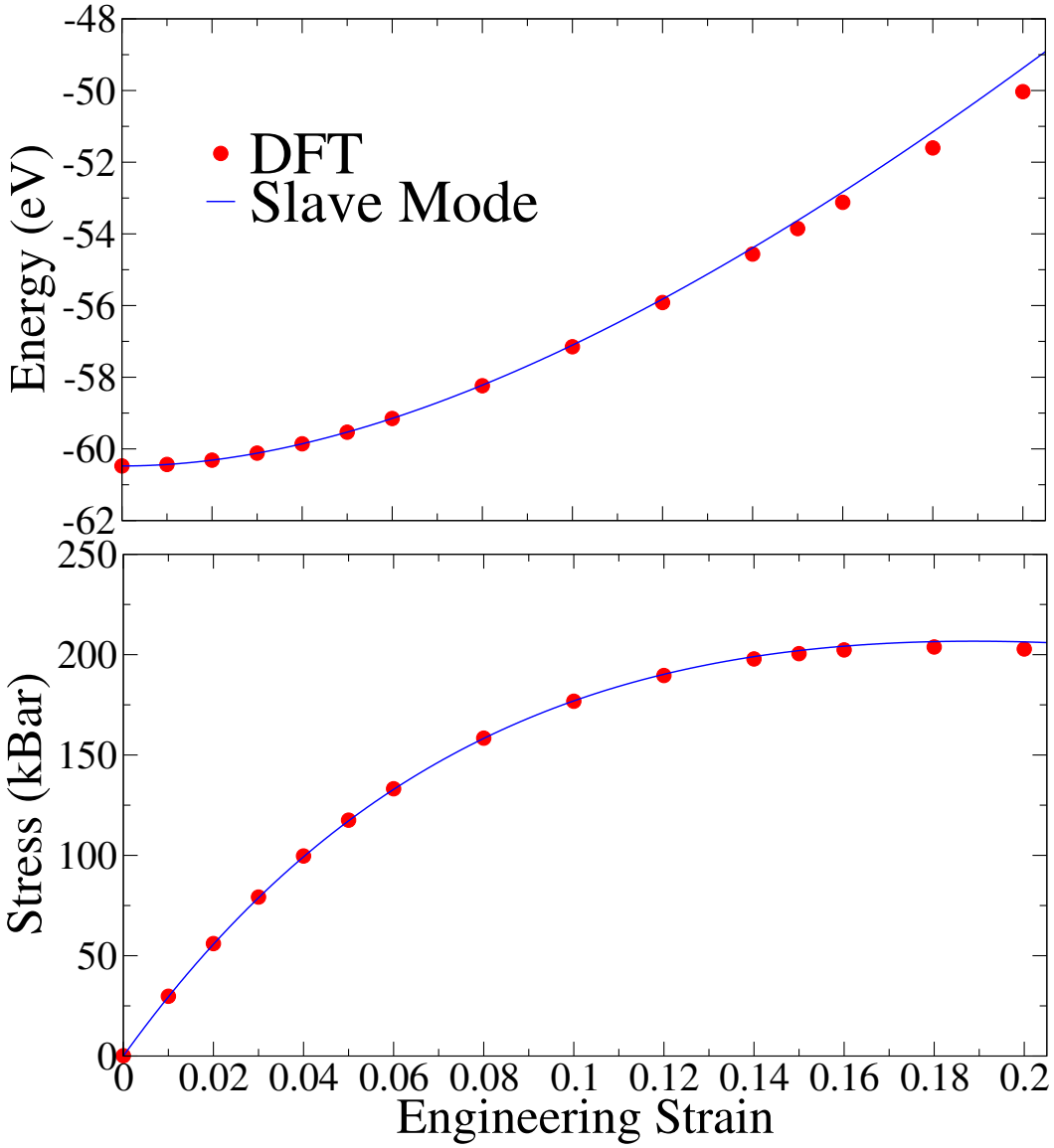

Figure 5.10: Energy and stress of graphene computed using slave mode expansion and DFT under strain

We also go to even higher strains up to 0.2 and one could observe from Fig. 5.14 that like the phonon softening process predicted by DFT, the potential up to 5th order drives down the phonons near Γ point and subsequently the K_1 mode at K point with strain.

The results could also be perceived from another point of view – for all strains, especially larger strains, 3rd order terms drive the K1 mode at K point down, 4th order terms drive it back up while 5th order terms drive it down again, indicating that the softening of K1 mode at K point is caused by the odd order terms in the potential. Because we only have terms within a hexagon in our potential, it is very promising that introducing terms within a bigger cluster would improve the prediction of K1 mode phonon softening a lot. What's more, even if that doesn't work, one might work on higher order terms, i.e. up to 7th order, for better performance.

"Armchair" Strain and "Zigzag" Strain

We also tried to strain the lattice along the "Armchair" direction and "Zigzag" direction, and the results are shown in Fig. 5.15 and Fig. 5.16. What could be observed from the predictions given by the potentials is that the degeneracy of the upper two branches at Γ point is lifted by these two kinds of strains, which is consistent with the underlying physics as the lattice symmetry is broken under these strains.

5.6 Conclusions

In conclusion, we have applied the slave mode expansion to generate the interatomic potential for graphene. We used a finite difference approach to compute the slave mode coefficients, and accurately determined all 93 terms – third and fourth order ones within a hexagon and fifth order dimer terms. Examining the energy, stress, and phonons under lattice strain indicates that our expansion is robust under a substantial strain of 0.05. When the strain is further increased, the phonon prediction results implies that terms within a bigger cluster may be needed for better performance. One could also go to higher order, i.e. 7th order, for even better improvements.

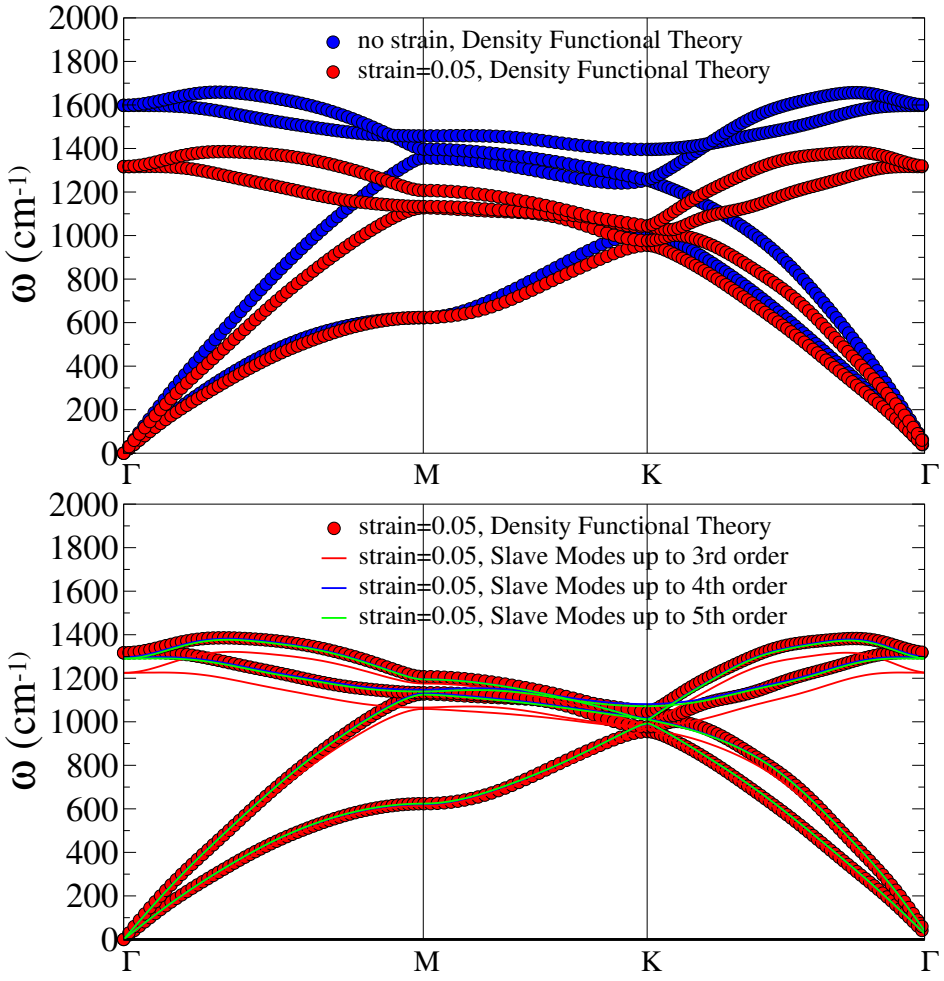

Figure 5.11: Phonon Dispersion of graphene under biaxial strain. Upper: the change of phonon dispersion under 0.05 strain, lower: comparison between phonon dispersions under 0.05 strain given by DFT and potentials up to each order.

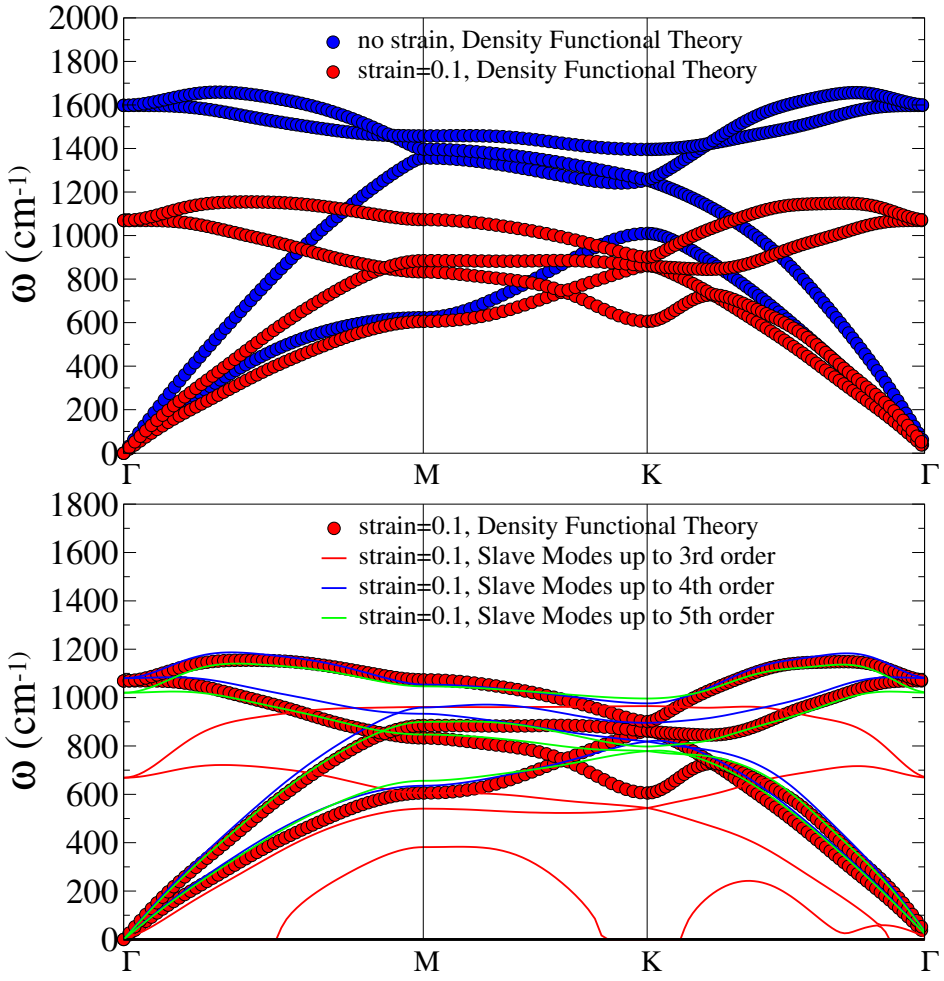

Figure 5.12: Phonon Dispersion of graphene under biaxial strain. Upper: the change of phonon dispersion under 0.1 strain, lower: comparison between phonon dispersions under 0.1 strain given by DFT and potentials up to each order.

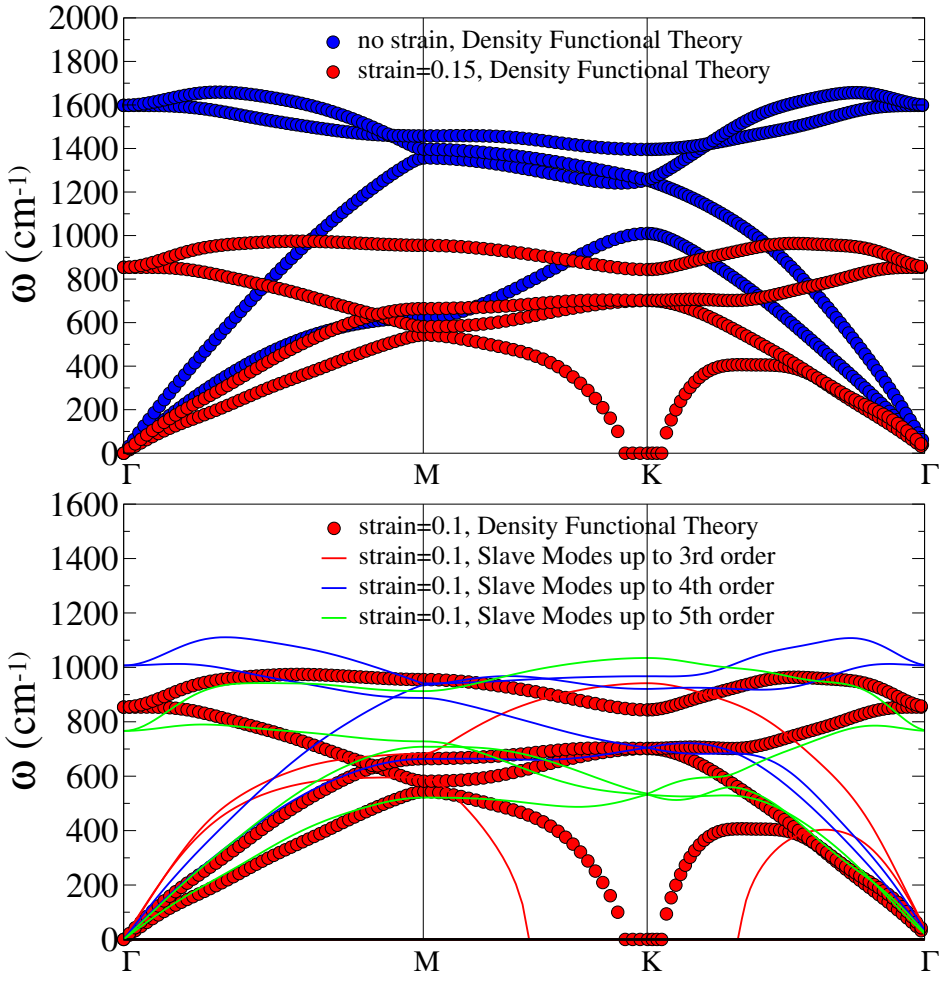

Figure 5.13: Phonon Dispersion of graphene under biaxial strain. Upper: the change of phonon dispersion under 0.15 strain, lower: comparison between phonon dispersions under 0.15 strain given by DFT and potentials up to each order.

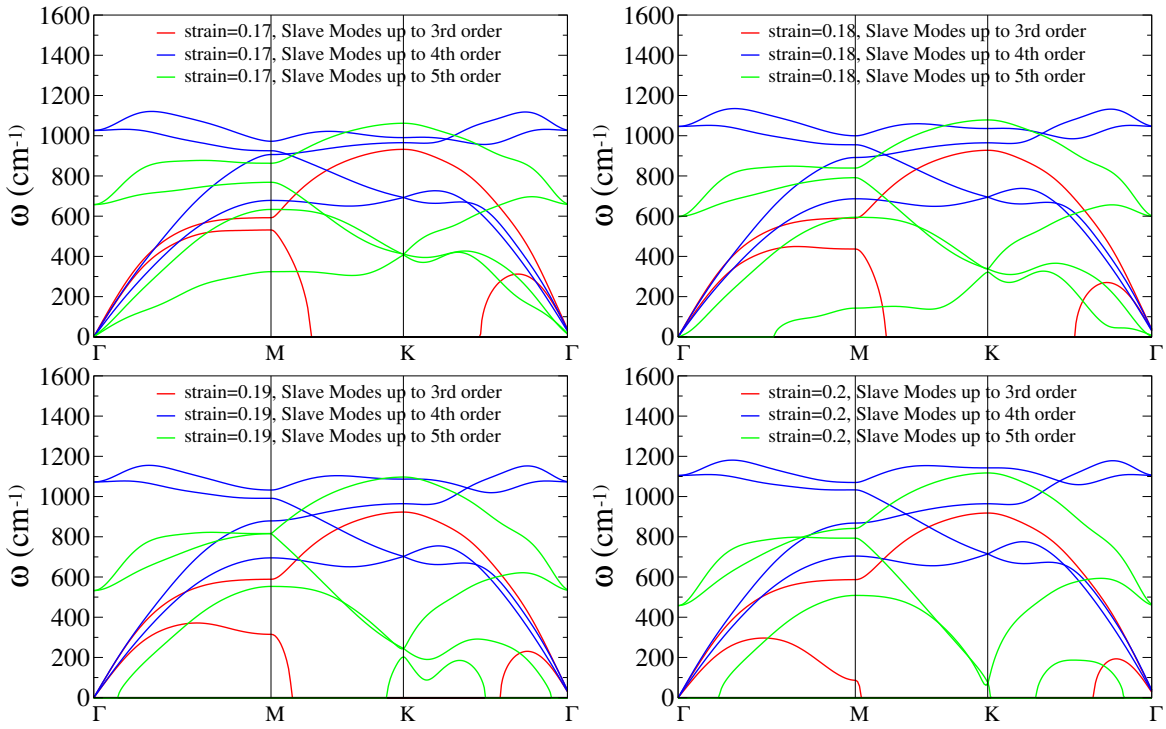

Figure 5.14: Phonon Dispersion of graphene under biaxial strain. Upper left: strain = 0.17, upper right: strain = 0.18, lower left: strain = 0.19, lower right: strain = 0.2.

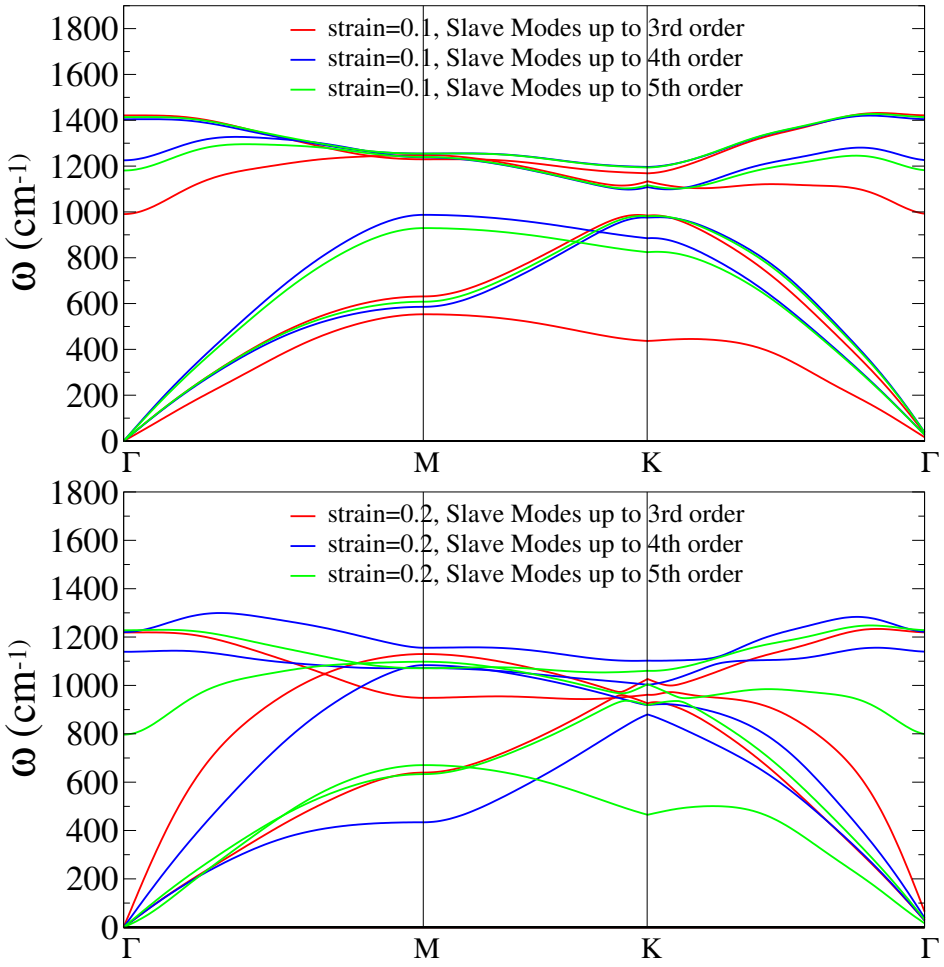

Figure 5.15: Phonon Dispersion of graphene under strain along armchair direction. Upper: 0.1 strain, lower: 0.2 strain

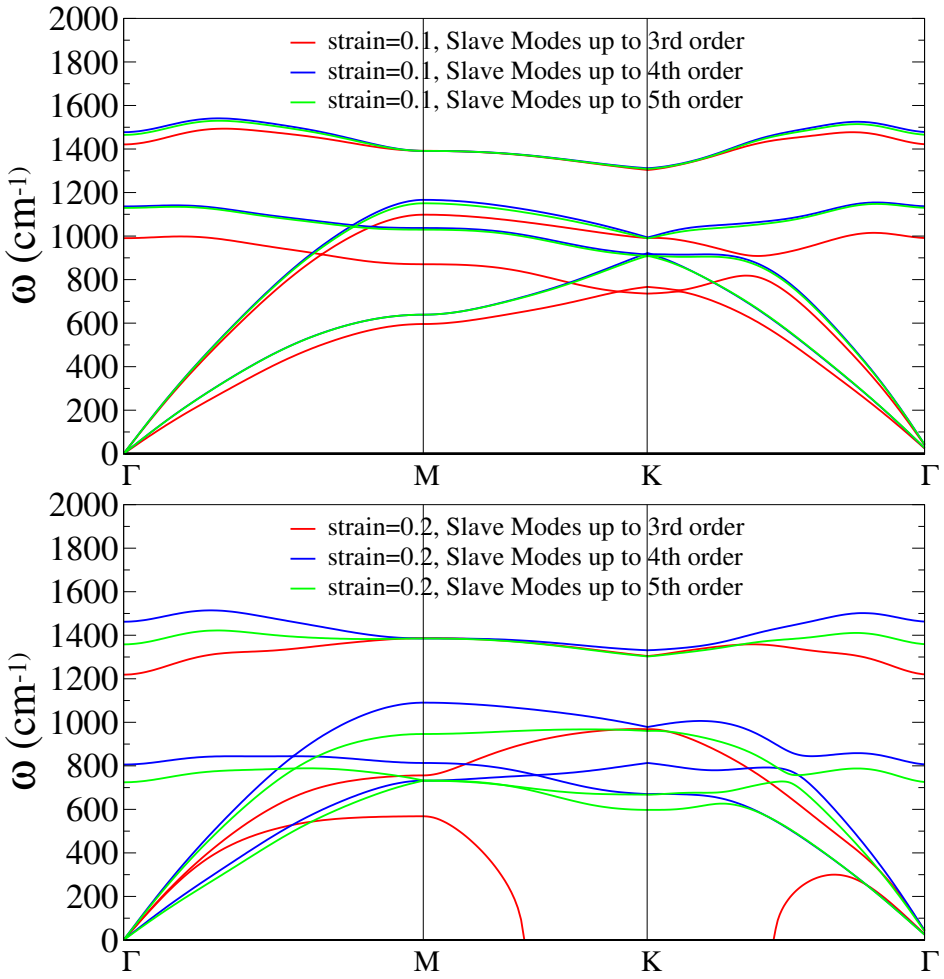

Figure 5.16: Phonon Dispersion of graphene under strain along zigzag direction. Upper: 0.1 strain, lower: 0.2 strain

Chapter 6

Summary

In this thesis, we worked on a new approach for constructing interatomic potentials, which are lattice energy functions of atomic displacements and enable accurate and efficient studies on material properties. Based on Taylor series expansion in terms of atomic displacement products, our approach has lattice symmetry - i.e. homogeneity of free space, group symmetry and lattice vector translational symmetry - imposed *a priori* and therefore not only has less parameters but also is free from the symmetry constraints when they are determined. In details, we used a set of variables - slave modes - instead of atomic displacements to expand the energies (achieved within Density Functional Theory) and the identities constructed in the product space of slave modes will constitute the expansion. Since slave modes are in fact atomic displacement modes, the slave mode expansion is actually a rearrangement of the Taylor series expansion in terms of atomic displacement products – indicating that the slave mode coefficients is also a rearrangement of the Taylor coefficients. Therefore, one could compute the Taylor coefficients using finite difference and then have them mapped into the slave mode coefficients via Singular Value Decomposition. We have shown that finite difference is reliable in computing the Taylor coefficients up to 5th order, though technical analysis is needed in investigating how it converges with Δ and supercell size.

We then applied the method and constructed a 4th order interatomic polynomial potential for PbTe with interactions constrained within an Octahedron and a 5th order interatomic polynomial potential for graphene with interactions constrained within a hexagon or a dimer. The potentials are then assessed in the way that they predict energy, stress and phonons under strain. It is found that the approach works well for PbTe since the potential constructed could not only reproduce its energy and stress up to a substantial strain but also give the right strain under which its TO mode phonon at Γ point becomes soft. However, it does not work so well for graphene – though it gives good energy and stress vs. strain, it is not able to give the right strain under which its K1 mode phonon at K point becomes soft.

Therefore, though we are confident that our expansion for PbTe is robust and the

terms outside of the octahedron are relatively small, we are not in the case of graphene. Possible reasons that our method does not work well there could be that its interactions is long-ranged and including terms within a hexagon only is not enough. What's more, it is also possible that one might need terms beyond 5th order to capture all the physics underlying the K1 mode phonon softening at K point in graphene. A detailed investigation using potentials up to 3rd, 4th and 5th order shows that the odd order terms softens the mode while the even order terms works in the opposite direction.

For future works, one might be interested in knowing whether the method is likely to work or not for a material before really applying it, or in other words, whether the approach is going to work for a material perfectly as in the case of PbTe or just so-so as in the case of graphene. There are a few tests one could carry out and some information one could collect before everything. For example, to determine the range of the interactions at a specific order, one could compute some Taylor coefficients corresponding to different coupling distances using finite difference and see how they decay. In addition, to estimate the order up to which one should expand the potential so that to investigate a phenomenon, one could take a look at the physical quantities associated. For instance, to investigate the phonon-softening of a material, one could analyze the stress-strain curve given by the right unit cell. In particular, one could fit the curve to the best order and that would be exactly one below the order of the potential.

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Appendix A

Generating Identities

The construction of terms in a slave mode expansion could be realized by the subroutines in `Construction.py`. A copy of this program could be found in the directory of `/home/ai/bin/main_codes/identity_generation` and a typical execution of this program is `python Construction.py path_to_scripts n`, with `path_to_scripts` being `/home/ai/bin` on soho, which indicates the location of some scripts it loads, and `n` being the order.[1] The following introduces how the subroutines in this program work.

The first subroutine creates some necessary input files based on point group theory using `representation.py`; among them there is `abs.pkl` which saves the symmetry operation matrices with basis being all atomic displacements within a cluster, `all.pkl` that saves the symmetry operation matrices with basis being slave mode representations derived within a cluster, and `cpdirrep.pkl` saving the slave mode representation as vectors in atomic displacement space.

The second subroutine creates some more input files that help when building the identities as well as $\mathcal{V}$ matrices. We mentioned in Chapter 2 and Chapter 3 that one has to make sure that all identities have to be linearly independent within an atomic cluster chosen as well as at the level of the lattice. To create these files, a `perturbonlattice`() object (e.g. `pbol`) designed in `clustermatch_final.py` is initialized. Thereafter `pbol.createlattice(mat, supa, visualization)` creates a big lattice. (Currently `'graphene'` and `'PbTe'` are accepted for `mat`; an example of `supa` would be `'9 0 0 0 9 0 0 0 1'`, and a lattice scaled by 9 in x and y direction would be created; and if `visualization` is `'true'`, the lattice created will be displayed.) With this lattice, the program is able to search for neighboring clusters that overlap with a given cluster. To achieve this, one first defines a `clusters` variable which is a dictionary of dictionaries, whose number depends on that of clusters chosen within a given unit cell, and each of the dictionaries are defined with keys being indexes of atoms in a

[1] The construction of dimer terms could be realized by `dimer_terms.py`, which could be found here – `/home/ai/Documents/group_theory`.

cluster and values being their coordinates in the lattice. In addition, one also needs to define a `clustersinlattice` variable which has the same structure with `clusters` but instead of using indexes of atoms within the cluster as keys, it use indexes of atoms within the lattice as keys – indicating that different atoms in the lattice is not going to share the same key. Next, one marks some atoms in the lattice so that the program could recognize the clusters overlapping with a given cluster by defining `disps`. Then, after running `pbol.markclusters(clusters, clustersinlattice)`, `pbol.displace(disps)` and `pbol.scan_match('irrep')`, two of the input files would be prepared - `iv_diff_dicts.pkl` and `iv_direct_dicts.pkl`. Finally, the third input file - `iv_inverse_dict.pkl` - is prepared after `pbol.ge_inverse_dict()`.

The third subroutine figures out the product space that contains identity by executing `allorderv.py`. The product spaces would be saved in `output_combs_`n`.pkl` with n being the order.

Last but not least, the subroutine creating the identities executes functions in `ivlist_lattice.py`. It takes in all the input files prepared above and creates an object `arangeiv()`, e.g. `iv`. Then, by running `iv.idbasis()` it would return the identities within cluster/clusters and identities within the lattice – the latter ones yield $\mathcal{V}$ matrices. The subroutine also creates `Xmatrice`n`.pkl` with n standing for the order, which is a numpy array of the matrice in Eqn. 3.1, and `sub_term`n`.pkl`, which is then transformed into tuples of numbers in `sterm`n`.pkl` that will be needed by `Parametrization.py` in Appendix B. In details, the transformation are done with the default mapping – $\{x_0 : 0, y_0 : 1, z_0 : 2, x_1 : 3, y_1 : 4, z_1 : 5, x_2 : 6, y_2 : 7, z_2 : 8, x_3 : 9, y_3 : 10, z_3 : 11, x_4 : 12, y_4 : 13, z_4 : 14, x_5 : 15, y_5 : 16, z_5 : 17, x_6 : 18, y_6 : 19, z_6 : 20, x_7 : 21, y_7 : 22, z_7 : 23, x_8 : 24, y_8 : 25, z_8 : 26, x_9 : 27, y_9 : 28, z_9 : 29, x_{10} : 30, y_{10} : 31, z_{10} : 32, x_{11} : 33, y_{11} : 34, z_{11} : 35\}$. For example, $(\mathtt{x_0}, \mathtt{x_0}, \mathtt{x_3})$ in `sub_term3.pkl` would be $(0, 0, 9)$ in `sterm3.pkl`.

Appendix B

Instruction on Monomial Coefficient Computing

The parametrization of a slave mode expansion could be accomplished by subroutines in `Parametrization.py` [1] [2]. In essence, it first prepares some input files so that the program could read forces from vasp output files automatically, then with `Xmatrice`n`.pkl` and `sub_term`n`.pkl` from `Construction.py`, it created some more input files. Next, directories of subdirectories in folder `POSCARs` for vasp runs are generated. After the runs are completed and moved to `vasp_runs_`n, monomial coefficients could be computed via finite difference and mapped back into slave mode coefficients via Singular Value Decomposition by the execution of `solve_term(material,n)` in `generatevasp_numrep.py`. Sometimes technical analysis on monomial coefficients is conducted so that less vasp runs will be required. One needs to know how they could be computed separately

[1] To repeat the parametrization of PbTe, one could find a copy of it in `/home/ai/Documents/group_theory/vasp_generate/PbTe_2_Octa_LS_dol` using `generatevasp_numrep.py` in the same directory. Because different representations have been used when constructing the potential (bond representation, slave mode representation and the mixture for minimal model), be careful about the input files. To repeat the parametrization for graphene, one could find a copy of it in `/home/ai/Documents/group_theory/vasp_generate/Graphene_Hex` using `generatevasp_numrep.py` in the same directory. For them, the input and output files are saved in `result` (see the rest of this appendix for details), and one needs to have the right files in `/home/ai/bin/temp` – do `cp mat/*.` with `mat` being `PbTe` or `graphene` in it. On the other hand, they could also be done with a more general one in `/home/ai/bin/main_codes/identity_parametrization` using a general `generatevasp_numrep.py` in `/home/ai/bin`. Its input files are saved in `inputs` and its output files are saved in `outputs`.

[2] The general one is able to create POSCAR files given one Δ or a range of Δs so that the whole process is automatic no matter one knows the optimal supercell size but needs to determine the optimal Δ after all runs are done as for graphene or is aware of both the optimal supercell size and Δ as for PbTe.

before carrying out the technical analysis and this will be introduced below.[3]

If one looks at Eqn. 3.5, it would be clear that a specific energy derivative could be computed from different force derivatives. For example, $\frac{\partial^3 E}{\partial^2 x_0 \partial x_3}$ could be computed from $\frac{\partial^2 F_3^x}{\partial^2 x_0}$ and $\frac{\partial^2 F_0^x}{\partial x_0 \partial x_3}$. For the first derivative, one needs to move atom 0 along x direction around and read the forces along x on atom 3 for finite difference, while for the second derivative, both atom 0 and atom 3 are moved around along x direction and forces along x on atom 0 are read. It means one could compute the monomial coefficients using the forces from one of the atomic displacement configurations or calculate the average after trying both of them. For convenience, we are going to call them finite difference from different configurations – in the given example, the first configuration is x_0x_0 and the second one is x_0x_3.

Therefore, before computing monomial coefficients using finite difference, one has to prepare some files so that the system knows all the configurations submitted and for a specific monomial, which configurations they could be computed from. To achieve all the files, one creates a folder named `result` in the same directory with script `generatevasp_numrep.py`[4]; one could then create subdirectories `num_rep` and `sym_rep` in `result` so that necessary input files and associated output files could be collected in them. To compute monomial coefficients, one needs to create a `sterm`n`.pkl` in `result/num_rep` instead of using the outputs from `Construction.py` as during parametrization. The same default mapping is used. For example, $\frac{\partial^3 E}{\partial^2 x_0 \partial x_3}$ would be $(0, 0, 9)$ in the list stored in `sterm3.pkl`

Then one executes `req_subterm(3,'test','')`[5] from `generatevasp_numrep.py` and the program is going to give three output files – `config3.pkl` storing configurations needed to compute all the monomial coefficients given in `sterm3.pkl`, `confsterm3.pkl` storing configurations and corresponding monomial coefficients they could compute and `stermconf3.pkl` storing monomial coefficients and configurations that they could be computed from. For our example, `config3.pkl` stores $[(0, 0)]$, `confsterm3.pkl` stores $\{(0, 0) : [(0, 0, 9)]\}$ and `stermconf3.pkl` stores $\{(0, 0, 9) : [(0, 9), (0, 0)]\}$. These files would be collected in `result/num_rep`.

Next, though it is not known what the optimal Δs and supercell sizes for finite difference calculation are, one needs to know the forces needed according to Eqn. 3.4. For our example, for $\frac{\partial^3 E}{\partial^2 x_0 \partial x_3}$ based on configuration x_0x_0, one needs forces $F_{3x}(x_0 = 2\Delta)$

[3] By going through them, one could also learn how the subroutines in `Parametrization.py` work.

[4] for these procedures, the one in either `/home/ai/Documents/group_theory/vasp_generate/Graphene_Hex` or `/home/ai/Documents/group_theory/vasp_generate/PbTe_2_Octa_LS_dol` would work.

[5] One could put some other number instead of 3 if working on a different order.

and $F_{3x}(x_0 = -2\Delta)$ since $F_{3x}(x_0 = 0)$ is 0. These forces should be computed in subdirectories within a folder named by the configuration and the subdirectories with all the VASP input files could be created by `posa_disp_dfd.py` or `posa_sc_dfd.py` after one executes `generate_all(material, 3)` from `generatevasp_numrep.py` (the program recognizes "`Graphene`" or "`PbTe`" for `material`) to generate another two files - `dir_vaspfile3.pkl` and `conf_vaspfile3.pkl`. In details, the first file stores configurations and the associated subdirectory names while the second one stores configurations as a tuple of numbers and the associated subdirectory names; for our example, the first file contains $\{'$`x0x0`$' : ['$`x0x0pp`$', 0, 0,'$ `x0x0mm`$']\}$ and the second file contains $\{(0, 0) : ['$`x0x0pp`$', 0, 0,'$ `x0x0mm`$']\}$.

Since `dir_vaspfile`n`.pkl` is usually used by `posa_disp_dfd.py` and `posa_sc_dfd.py` for subdirectory preparation or `fd_disp_dfd.py` and `fd_sc_dfd.py` for finite difference calculation, which are currently collected in `/home/ai/bin`, it is collected in `/home/ai/bin/temp`. On the other hand, `conf_vaspfile`n`.pkl` is usually used by `generatevasp_numrep.py` for finite difference calculation and is therefore collected in `result/num_rep`.

In more details, `posa_disp_dfd.py` or `posa_sc_dfd.py` create the subdirectories with all the VASP input files for force computation within directories classified by Δ and supercell size in a folder named by the configuration. A selection of Δs, a supercell size and the material name are provided in `posa_disp_dfd.py`. For our example, if $[0.035, 0.05, 0.07]$ are provided for Δs, directories `disp_0.035`, `disp_0.05` and `disp_0.07` will be created in the folder named `x0x0`, and subdirectories `x0x0mm` and `x0x0pp` with `INCAR`, `POTCAR`, `KPOINTS` and corresponding `POSCAR` will be prepared in each of them. On the other hand, a selection of supercells, a Δ and the material name are provided in `posa_sc_dfd.py`. For our example, if $[(8, 8, 1), (9, 9, 1)]$ are provided, directories `SC_8_8_1` and `SC_9_9_1` will be created in `x0x0`, and subdirectories `x0x0mm` and `x0x0pp` with `INCAR`, `POTCAR`, `KPOINTS` and corresponding `POSCAR` will be prepared in each of them. One would notice that the programs could recognize the coordinates of an atom by simply knowing its index – this is not magic but information stored in `/home/ai/bin/temp/sc_atom_pos.pkl`, which is created by running `/home/ai/bin/sc_atom_pos_nr.py`.

Then one could submit all the runs from the subdirectories and the finite differences vs. Δ or supercell size could be computed in the folder named by the configuration by running `fd_disp_dfd.py` or `fd_sc_dfd.py`. For the specific $\frac{\partial^3 E}{\partial^2 x_0 \partial x_3}$, the commands are `python fd_disp_dfd.py x 3 supercell size`[6] or `python fd_sc_dfd.py x 3`[7]

[6] supercell size could also be provided in the script

[7] Δ has to be provided in the script

in folder `x0x0`. These programs uses `/home/ai/bin/temp/sc_atom_nr.pkl` created by `/home/ai/bin/sc_atom_pos_nr.py` to read the forces from the right lines in `OUTCAR`. In addition, sometimes one might also be interested in comparing the forces when different supercells are used. This is possible with `/home/ai/bin/test_sc_dfd.py`[8]; Δ and the two supercell sizes to be compared are provided in this script.

The last things to mention in this appendix, for parametrization of a slave mode expansion, though `Parametrization.py` takes in `Xmatrice`n`.pkl` and `sterm`n`.pkl` provided by the subroutines in `Construction.py` mentioned in Appendix A by default[9], it is also possible to generate those files if all the terms and appropriate subterms are provided. In addition, the vasp runs have to be in a specific directory (`vasp_runs` for PbTe and `vasp_runs_`n for graphene) in the same directory with `Parametrization.py` during the parametrization process so that the program could read the forces from the right place and compute the monomial coefficients. For PbTe, after the optimal Δs and supercell sizes are determined, the subdirectories are moved to `vasp_runs`. For graphene, because the optimal Δs need to be determined for different cases[10], which is automated in the program, the folders named by configurations with directories containing subdirectories generated using different Δs are moved to `vasp_runs_`n.

[8] The program uses `/home/ai/bin/temp/sc_atom_pos_test.pkl` created by `/home/ai/bin/sc_atom_pos_nr_test.py` to recognize the same atom from different supercells.

[9] They should be put in the same directory, which is `inputs`, which is in the same folder with `Parametrization.py`.

[10] Those for third order are incorporated in the code, but those for 4th and 5th order could be determined again

Appendix C

Correction on K matrices

We mentioned in Chapter 3 that we used two Octahedra when deriving the terms for PbTe, one centered on Pb and the other centered on Te. These two Octahedra are given in Fig. C.1 with atoms indexed. Because the interactions between Octahedra are not considered, the two Octahedra could be located anywhere; and for conveniency, especially when constructing the $\mathcal{V}$ matrices, the two in the Figure are chosen. One

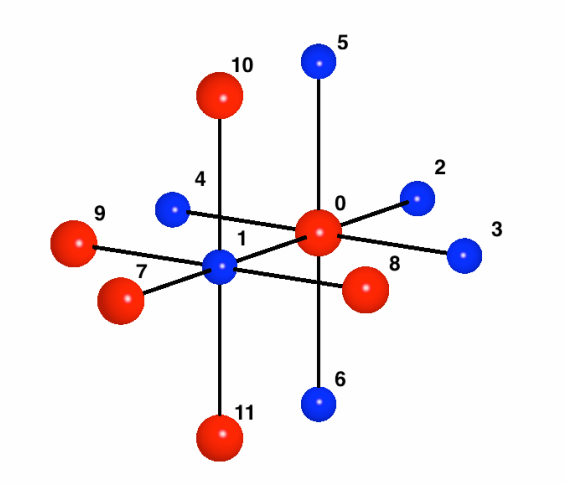

Figure C.1: The indexes of the atoms within the two Octahedra we use.

could figure out what interactions the monomial terms stand for with this plot.

On the other hand, when PbTe's lattice is strained, one has to renormalize its harmonic coefficients with the anharmonic terms so that to correct its K matrices and recompute its phonon dispersion. With this plot, we could clarify that process. For example, the 3rd order term in the minimal model within an Octahedron could be written down as follows –

$$T^3_\sigma(R=0) = (x_1-x_0)^3 - (x_2-x_0)^3 + (y_3-y_0)^3 - (y_4-y_0)^3 + (z_5-z_0)^3 - (z_6-z_0)^3, \tag{C.1}$$

and the final term in the potential contributed by the two Octahedra will be –

$$\begin{aligned}\sum_R T^3_\sigma(R) = {} & x_0^2x_1 - x_0x_1^2 - x_0^2x_2 + x_0x_2^2 + x_1^2x_7 - x_1x_7^2 \\ & - x_{10}^2x_5 + x_{10}x_5^2 - x_{11}^2x_6 + x_{11}x_6^2 + x_3^2x_8 - x_3x_8^2 \\ & + x_4^2x_9 - x_4x_9^2 + y_0^2y_3 - y_0y_3^2 - y_0^2y_4 + y_0y_4^2 \\ & + y_1^2y_8 - y_1y_8^2 - y_1^2y_9 + y_1y_9^2 + z_0^2z_5 - z_0z_5^2 \\ & - z_0^2z_6 + z_0z_6^2 + z_1^2z_{10} - z_1z_{10}^2 - z_1^2z_{11} + z_1z_{11}^2.\end{aligned} \tag{C.2}$$

When the lattice is strained, this term is going to renormalize the harmonic coefficients associated with onsite interactions and each of the couplings within the two Octahedra – nearest Pb-Te, nearest Pb-Pb, nearest Te-Te, next nearest Pb-Pb, next nearest Te-Te because it will yield corrections on them. For instance, if the lattice is strained along x direction by engineering strain e, x_0 doesn't change while x_1 becomes $x_1 + be$ with b being the length of Pb-Te bond. The component of $x_0^2x_1 - x_0x_1^2$ in this term would then renormalize the onsite x_0^2 interaction by be and the nearest neighbor x_0x_1 coupling by $-2be$ because $[x_0^2(x_1+be) - x_0(x_1+be)^2] - [x_0^2x_1 - x_0x_1^2] = x_0^2be - 2bex_0x_1 - x_0b^2e^2$ and $-x_0b^2e^2$ is not a correction. The corrections given by the other components in this term could be achieved similarly.

To discuss how the K matrices are corrected, we will introduce how they are defined first. For a d dimensional system with n atoms in one unit cell, the K matrices are usually nd by nd and they are indexed by translational vectors $\mathbf{R}$s. In essence, K($\mathbf{R}$) is going to be stacked up by n^2 d by d submatrices. The submatrices are d by d because each of them has the d^2 harmonic coefficients between two atoms. Because the submatrices are stacked on rows and columns, we could refer to them using index (i, j) with i standing for the row number and j standing for the column number. The (i, j)th submatrice of K($\mathbf{R}$) will then record these harmonic coefficients between the ith atom in one unit cell and the jth atom in the unit cell translated from the previous one by $\mathbf{R}$.

For PbTe, we will have 6 by 6 K matrices that are stacked by four 3 by 3 submatrices recording from upper left to lower right the harmonic coefficients of xx, xy, xz, yx, yy, yz, zx, zy and zz couplings. In details, the $(1,1)$ submatrice would record the harmonic coefficients between Pb in one unit cell and Pb in the other translated by $\mathbf{R}$, with the upper left entry being the coefficient of $x_{Pb}x_{Pb}$; and the $(1,2)$ submatrice would record the harmonic coefficients between Te in the first unit cell and Pb in the second unit cell, with the upper left entry being the coefficient of $x_{Te}x_{Pb}$, and etc. Thus, bex_0^2 from above is going to impose a correction with value be on the upper left entry of the $(1,1)$ submatrice of $K(0,0,0)$, while $-2bex_0x_1$ is going to impose a correction with value $-2be$ on the upper left entry of the $(1,2)$ submatrice of $K(0,-1,0)$ and the upper left entry of the $(2,1)$ submatrice of $K(0,1,0)$.

For Graphene, the correction on K matrices could be dealt with in a similar manner and the one only needs to be careful when figuring out which K matrices are affected when renormalizing a bond.

Therefore, according to the aforementioned procedures, the corrections on K matrices could be taken care of and saved as a dictionary with keys being $\mathbf{R}$ and values being the correction matrice on the corresponding K matrice in a `.pkl` file[1] after executing `correct_mat(strain)` from `generatevasp_numrep.py`. With correction files available, `phonons.py`[2] is then able to generate phonon dispersions under strains. In details, the data would usually be stored in a file called `bands.out` and one could visualize them with some simple python codes (e.g. those in `plot.py`[3]). Plots that meet the standard of publications could also be generated using `gracey.py`.

[1] An example could be found here – `/home/ai/Documents/group_theory/vasp_generate/Graphene_Hex/result/num_rep/correction_3`.

[2] It is a script that computes the harmonic force constants using the finite displacement method; and one could find an example here – `/home/ai/Documents/projects/graphene/phonons/nostrain/881_supa_k3_acc_hc_nrp`.

[3] A copy could be found here – `/home/ai/Documents/projects/graphene/phonons`.

Appendix D

Monomial Coefficients for PbTe

The monomial coefficients computed for parameterizing PbTe's potential are listed in the tables below.

Table D.1: Monomial coefficients for 3rd order terms of PbTe

monomial	coefficient	monomial	coefficient	monomial	coefficient	monomial	coefficient
$x_2z_0z_6$	-0.175	$z_1z_3z_5$	-0.02	$z_5z_6^2$	-0.288	$x_1x_2z_6$	0.162
$x_1z_3z_4$	-0.008	$x_7^2y_9$	0.134	$x_1z_6^2$	-0.061	$y_4z_4z_6$	-0.17
$x_{10}z_{10}z_7$	-0.115	$x_2z_0z_2$	0.24	$z_3^2z_5$	-0.029	$x_2z_0z_3$	0.03
$y_1z_3^2$	-0.025	$x_8z_{10}z_7$	0.005	$y_0z_0z_4$	-0.005	$y_{10}z_7z_9$	-0.002
$y_3y_6z_4$	0.008	$x_{10}x_{11}x_7$	-0.015	$z_1z_2z_6$	0.008	$y_2z_0z_3$	0.013
$x_1z_2z_4$	0.005	$x_4y_6z_2$	0.005	$x_1x_7z_{10}$	0.265	$x_9z_7z_9$	0.018
$x_{11}z_0z_{10}$	-0.018	$x_1z_3z_6$	0.005	$x_{11}^2z_7$	-0.129	$x_4x_6y_6$	-0.007
$x_2z_1z_2$	-0.027	$x_0x_9z_{10}$	0.01	$x_1x_9z_{10}$	-0.062	$x_1x_{10}z_{10}$	-0.077
$z_0z_4z_6$	-0.064	$x_8y_{11}z_7$	-0.0	$x_{10}^2z_9$	-0.037	$x_{10}x_{11}y_8$	-0.008
$x_0x_{10}x_9$	-0.01	$x_{10}x_9y_8$	-0.013	$y_6z_3z_6$	-0.165	$x_1x_{10}z_{11}$	0.222
$z_0z_6^2$	-2.821	$y_0z_3^2$	-0.056	$x_2z_1^2$	-0.091	$x_{10}y_8z_0$	0.01
$x_2y_3z_5$	-0.027	$x_2z_1z_5$	0.026	$x_9z_7z_8$	-0.0	$x_1x_9y_{11}$	0.015
$x_{10}x_9z_{10}$	-0.023	$x_{10}x_7z_{11}$	-0.012	$x_{10}x_{11}z_{10}$	0.062	$x_1^2z_{11}$	-0.009
$x_{10}^2z_1$	-0.15	$x_1x_7^2$	2.874	$y_6z_3^2$	0.061	$y_3z_0z_4$	-0.345
$x_1x_{10}x_7$	0.019	$x_{10}^2z_{11}$	-0.0	$x_2y_5z_3$	-0.005	$x_4z_1z_3$	0.0
$x_1z_0z_{10}$	-0.039	$x_7y_8y_9$	-0.148	$x_{11}^2x_7$	-0.005	$y_0y_5z_3$	0.043
$x_1^2x_7$	-2.819	$x_0x_{10}z_{10}$	0.106	$x_0x_7^2$	0.027	$x_{11}^2y_9$	-0.035
$y_3y_6z_0$	-0.017	$x_0y_9z_{10}$	0.058				

Table D.2: Monomial coefficients for 4th order terms of PbTe

monomial	coefficient	monomial	coefficient	monomial	coefficient	monomial	coefficient
$y_0y_{10}y_{11}y_8$	0.005	$z_1z_{10}^2z_{11}$	-0.611	$x_1x_{10}y_8z_{11}$	0.057	$x_8y_0z_0z_9$	0.008
$x_0x_7y_{11}z_8$	-0.01	$y_9z_{10}^2z_8$	0.007	$y_{10}y_{11}y_9z_{10}$	-0.027	$x_5x_6z_2^2$	-0.007
$x_1x_6z_2^2$	-0.003	$x_1x_4y_5^2$	0.003	$x_{11}x_7y_{10}^2$	0.005	$z_{10}z_{11}^2z_8$	-0.02
$y_1^2z_2^2$	0.085	$x_0^2y_5^2$	0.011	$z_1^2z_{11}z_9$	-0.04	$x_1x_2^2x_5$	0.024
$x_1x_{11}x_7z_1$	0.05	$x_0x_8y_{10}^2$	-0.003	$x_0^2x_1z_6$	-0.183	$y_4z_1z_2z_6$	0.001
$y_9z_1z_{11}z_9$	0.034	$y_0y_1y_{10}y_{11}$	0.039	$x_1^2y_5z_3$	-0.005	$x_4y_1^2z_5$	0.001
$x_0^2y_2y_4$	0.112	$x_6z_0z_1^2$	-0.077	$y_9z_{10}^2z_{11}$	0.035	$x_3x_5y_3z_0$	0.007
$y_{10}y_8z_{10}z_9$	0.025	$y_9^2z_1z_{10}$	-0.1	$x_0^2z_0z_3$	0.015	$z_1z_{11}z_9^2$	0.056
$x_0^2y_4y_5$	-0.02	$x_7y_1z_0z_9$	0.008	$x_0^2z_1z_3$	-0.019	$x_{11}y_0y_8z_{11}$	-0.003

$x_3y_6z_2z_3$	0.004	$z_1^2z_6^2$	0.024	$x_1x_3x_6z_4$	-0.0	$x_3x_6y_1y_5$	0.001
$x_0^3x_5$	-0.07	$x_{11}x_7y_{11}z_8$	-0.001	$x_7^2z_1z_7$	0.723	$x_3y_1z_4^2$	-0.003
$x_{10}x_{11}z_{11}z_9$	0.005	$y_{10}y_{11}z_8z_9$	0.004	$z_2z_3z_6^2$	-0.006	$x_2y_5z_2z_4$	0.008
$z_7z_8^3$	0.015	$x_3x_6z_0z_6$	0.017	$x_4x_6y_6z_5$	-0.003	$x_{11}x_8y_{10}z_9$	0.005
$x_2y_4z_2z_4$	0.02	$x_2y_2^2y_4$	0.123	$x_0^2x_5z_2$	0.021	$y_0z_{11}^2z_8$	0.001
$x_5^2x_6z_2$	0.007	$x_7^2z_7z_9$	-0.003	$y_0y_{10}y_{11}y_7$	0.025	$z_0^2z_8z_9$	0.031
$x_2x_6y_0z_4$	-0.004	$x_2y_2z_2z_3$	0.052	$y_0y_1z_0z_1$	0.041	$x_0y_8z_7^2$	-0.02
$y_8y_9z_0z_8$	-0.005	$y_0y_{10}y_7z_9$	-0.002	$x_0x_5y_4y_5$	0.006	$x_8y_9z_7z_8$	-0.001
$x_1^3z_5$	0.015	$y_{10}y_9z_{10}^2$	-0.047	$x_1^2z_1z_3$	0.002	$y_8y_9z_0^2$	-0.001
$x_0x_1z_9^2$	0.032	$y_1z_{10}z_9^2$	0.003	$x_5z_2z_3z_6$	-0.0	$x_0x_8y_{10}y_{11}$	0.0
$y_1y_2y_3y_6$	-0.003	$z_{10}^2z_8^2$	-0.042	$x_0^2y_1y_2$	0.019	$x_0^2y_2^2$	-0.452
$x_4y_0y_2y_5$	0.004	$y_{10}y_9z_1z_9$	-0.068	$x_0y_1z_1z_4$	-0.013	$x_0z_1^2z_{11}$	0.011
$x_5^2z_0z_6$	-0.073	$x_0x_6y_3z_0$	0.078	$y_2^3y_4$	-0.01	$x_0y_2z_0z_3$	-0.002
$x_6z_1^2z_6$	0.071	$x_7z_{10}^2z_7$	-0.044	$y_1y_9z_1z_{10}$	0.371	$x_5^2z_5z_6$	0.273
$z_0z_1^2z_2$	-0.001	$x_1x_5z_6^2$	-0.007	$x_4y_1z_2z_3$	-0.001	$y_1y_{10}z_8z_9$	0.035
$y_2^2z_2z_3$	0.001	$y_0y_1z_9^2$	0.015	$x_1^2z_5^2$	0.01	$z_{11}z_8z_9^2$	0.009
$x_0x_6y_5^2$	-0.03	$x_5y_2y_6z_0$	0.002	$x_7y_1y_{11}y_9$	-0.012	$x_3y_2z_0z_6$	-0.003
$x_1z_1z_6^2$	0.072	$x_0x_4y_0y_2$	0.073	$x_0x_1^2z_6$	0.1	$y_{10}^2z_7^2$	-0.028
$y_0y_9z_0z_8$	-0.002	$x_5x_6z_6^2$	-0.011	$y_0y_{10}y_8z_9$	-0.001	$x_6z_0z_2z_6$	-0.034
$z_0z_1z_7^2$	-0.06	$y_0y_{10}z_{10}z_8$	0.001	$y_9^2z_0z_7$	0.012	$x_7^2z_0^2$	0.026
$x_0y_7z_1z_8$	0.005	$x_0^2z_3z_4$	0.007	$x_0x_5y_5^2$	-0.007	$x_2y_4z_1z_3$	0.003
$z_0z_7^3$	0.034	$x_{10}z_0z_8^2$	-0.002	$x_1x_9z_1z_8$	0.085	$x_1x_{11}z_{11}z_9$	0.034
$y_2y_4z_1z_6$	0.006	$x_6y_2z_4z_6$	0.005	$x_0x_{10}x_{11}y_8$	0.004	$x_7y_{10}y_8z_{11}$	-0.007
$x_0x_{10}y_{11}y_9$	0.001	$z_1^2z_{10}z_{11}$	0.804	$x_1x_7z_0z_8$	0.004	$x_{10}x_{11}y_0y_7$	0.01
$y_{10}y_8z_{10}z_8$	0.261	$x_1x_6z_2z_6$	0.043	$x_0^2x_3x_4$	0.085	$y_1^2y_5^2$	0.018
$x_7z_{10}z_7^2$	-0.015	$y_{10}y_9z_1z_{10}$	-0.073	$x_0y_0y_{11}z_8$	0.004	$y_{10}z_1z_{10}z_8$	0.0
$x_1x_7z_0z_1$	0.189	$x_1^2z_1^2$	-1.595	$x_9y_0y_{11}z_{10}$	-0.001	$y_{11}y_7z_7z_9$	0.006
$x_{11}z_7^3$	0.022	$y_{10}y_7z_0z_9$	0.007	$z_0z_1z_9^2$	-0.014	$x_1y_1y_4z_6$	-0.007
$x_0x_4z_5z_6$	0.036	$z_1^3z_7$	-0.026	$x_0^2y_6z_3$	0.009	$x_0x_1^2x_2$	-0.523
$x_0z_1z_6^2$	-0.01	$z_{10}^3z_8$	-0.007	$x_8x_9y_{10}z_9$	0.004	$x_0x_6z_3z_4$	-0.0
$x_1x_9z_1^2$	-0.013	$x_0^2x_5^2$	0.052	$x_9^2z_0z_8$	-0.005	$x_{10}x_{11}y_7^2$	0.002
$x_1y_1y_2y_4$	-0.018	$x_0x_4y_4y_5$	0.016	$x_1x_6^2z_0$	0.017	$x_7y_9z_7z_8$	-0.011
$x_1x_7z_0^2$	-0.086	$y_0^2z_8z_9$	0.005	$y_2^2z_2^2$	-1.586	$y_1y_2z_1z_2$	0.017
$y_2y_4z_1z_3$	-0.003	$y_{11}y_9z_{10}z_7$	-0.001	$x_7^2z_7^2$	-1.137	$y_1y_{10}z_1z_9$	0.032
$x_0x_6y_4z_4$	-0.004	$x_2x_6z_5z_6$	-0.038	$z_1z_2z_3z_4$	-0.001	$x_0x_2x_6y_4$	0.006
$x_1y_8z_7^2$	0.042	$z_1^2z_2^2$	0.03	$x_0x_4z_1z_3$	-0.004	$x_4x_6y_1z_1$	0.0
$x_1^3x_6$	-0.015	$z_0z_2z_5z_6$	-0.204	$x_1^2z_1z_6$	-0.097	$z_1z_{10}^3$	-3.951
$x_1y_3z_0z_1$	0.039	$x_{10}x_{11}y_{10}y_7$	0.01	$x_{10}y_7^2z_0$	0.012	$x_0y_9z_0z_9$	0.015
$x_{11}y_0z_0z_9$	0.001	$x_0x_7z_0z_7$	0.07	$x_1x_{11}z_8z_9$	-0.001	y_2^4	1.769
$x_7y_1z_1z_9$	0.141	$z_1^2z_8z_9$	0.133	$x_2y_2y_4y_6$	-0.002	$z_0z_1z_3z_4$	-0.035
$x_0x_7z_{11}z_8$	-0.008	$y_0z_{11}z_9^2$	0.0	$x_5z_1z_5z_6$	-0.002	$x_3x_6z_3z_6$	-0.027
$y_9^2z_1z_7$	0.028	$y_2^2z_5z_6$	-0.029	$x_{11}x_7y_1y_9$	0.026	$x_1x_4y_5z_4$	-0.007
$x_0x_3y_5^2$	-0.003	$x_7y_7z_0z_8$	-0.003	$x_4x_6z_3z_6$	0.004	$x_1x_7z_0z_{11}$	-0.013
$x_0y_2y_6z_0$	-0.013	$x_5x_6z_1z_2$	0.004	$x_5x_6y_4z_5$	-0.009	$x_9y_0z_0z_1$	0.028
$z_0z_1z_{10}z_{11}$	0.019	$y_{11}y_9z_{10}^2$	-0.004	$z_1^2z_2z_3$	-0.003	$x_1x_6z_1z_6$	0.414
$x_{11}x_9z_{11}z_9$	-0.038	$z_{10}^2z_{11}^2$	0.219	$x_0x_6z_5z_6$	-0.281	$x_4y_1y_5y_6$	0.001
$x_1x_2z_5z_6$	0.004	$z_{10}^3z_{11}$	0.297	$x_0x_3y_4y_5$	-0.004	$x_3x_6z_1z_2$	0.001
$x_1x_9z_0z_8$	0.001	$y_{10}y_7z_7^2$	-0.005	$x_0x_2y_2y_4$	-0.075	$x_0y_9z_0^2$	-0.138
$y_1y_{11}z_9^2$	-0.031	$x_7z_{11}^2z_9$	-0.025	$x_0^2z_5z_6$	0.495	$y_3z_1^2z_6$	0.0
$x_0x_1^2x_6$	0.042	$x_0x_5z_2z_6$	-0.044	$x_9y_0z_1z_{10}$	-0.006	$x_1x_5z_3z_6$	-0.002
$z_1z_{10}^2z_7$	0.061	$x_0^2z_0z_6$	0.356	$y_2y_4z_2z_3$	-0.005	$x_1z_0z_1z_6$	0.05
$x_0^2x_4x_5$	0.0	$x_0x_7z_1^2$	0.326	$z_0z_1z_4z_6$	-0.011	$y_{11}y_9z_{10}z_8$	-0.001
$x_7y_{10}^2z_7$	0.012	$y_0y_{11}z_{10}z_8$	0.002	$x_6y_4z_0z_1$	-0.002	$x_0x_1z_1z_9$	-0.082
$y_9z_{10}^3$	0.021	$y_1y_2z_2^2$	0.046	$x_4x_6z_5z_6$	0.001	$x_0y_0z_0z_8$	0.075

$x_6z_2z_6^2$	0.128	$z_0z_8^2z_9$	0.007	$x_2^2x_6z_4$	-0.004	$x_1^2x_2z_5$	0.042
$x_6y_4z_1z_6$	0.005	$y_1y_{11}y_9z_{10}$	0.032	$x_6^2z_4z_6$	0.033	$x_1y_2z_1z_3$	-0.001
$x_2^2y_4z_5$	0.01	$y_{10}y_7y_9z_7$	-0.007	$y_8y_9z_0z_7$	0.008	$y_1^2y_5z_4$	0.002
$x_{10}x_7^2z_0$	0.01	$x_8y_{10}y_9z_7$	0.001	$z_1z_4^2z_6$	0.005	$x_6^2y_1z_4$	0.002
$x_8y_7z_1^2$	-0.014	$x_4x_6y_5z_5$	-0.001	$x_{11}y_8z_7^2$	-0.012	$x_1y_4z_2z_4$	0.008
$x_4x_6^2z_1$	0.002	$x_4y_2^3$	0.016	$x_0x_{10}y_9z_0$	0.006	$x_5x_6z_2z_5$	0.001
$x_4y_1z_2z_5$	0.001	$x_1x_9z_8z_9$	-0.031	$x_0y_9z_{11}z_9$	-0.007	$x_5x_6y_1y_2$	-0.004
$x_{11}x_7z_0z_7$	-0.011	$z_1z_{10}z_8z_9$	-0.011	$x_0x_7y_8z_{11}$	-0.024	$x_1y_7z_1z_9$	0.026
$x_1x_3y_2y_4$	0.002	$x_1y_4y_6z_2$	-0.001	$x_{10}y_8z_0z_{11}$	-0.009	$y_2^2z_3^2$	-0.019
$x_0x_1x_6z_0$	-0.04	$x_0y_7z_0z_8$	0.002	$x_1y_7z_{11}z_9$	0.003	$x_0x_4y_0y_5$	-0.003
$z_0z_{10}^2z_7$	0.021	$y_0^2z_0z_1$	0.016	$z_{10}z_{11}z_7^2$	-0.021	$x_{11}x_7z_1^2$	0.04
$x_0^2y_0y_2$	0.741	$x_1x_{10}z_9^2$	-0.003	$x_2x_3z_1^2$	0.007	$y_0^2z_0z_7$	0.02
$y_7y_8z_0z_8$	0.001	$x_7y_1z_{11}z_9$	-0.016	$x_1^2y_0y_5$	0.016	$x_3x_6y_6z_3$	-0.011
$x_0x_2z_5z_6$	-0.216	$x_1x_7z_7^2$	0.369	$z_1^2z_{10}^2$	5.403	$z_{10}z_7z_8^2$	0.012
$x_0x_3z_0z_3$	0.046	$x_2z_1z_4z_6$	-0.001	$x_1^2x_6z_2$	-0.005	$y_1y_2^3$	-0.004
$y_0y_1z_0z_8$	0.004	$x_7x_9z_0z_8$	0.0	$y_0y_7z_0z_7$	0.027	$x_4x_5y_2y_5$	-0.001
$y_{11}^2y_7z_9$	-0.001	$x_0y_9z_1z_{10}$	0.014	$x_4y_1z_5z_6$	0.001	$x_1x_5y_2z_3$	0.001
$x_1y_7z_0z_9$	0.001	$x_6y_1y_4z_6$	0.008	$x_4x_6z_2z_5$	0.0	$x_4y_1y_6z_5$	-0.0
$y_8y_9z_0z_1$	0.032	$y_9^2z_{10}^2$	0.037	z_1^4	1.774	$x_0x_{10}y_{10}y_9$	-0.0
$z_1^3z_{10}$	-3.605	$z_0z_{10}z_{11}z_7$	-0.001	$x_1y_{10}y_7z_7$	0.014	$x_1^2y_0y_2$	0.082
$y_9^2z_7z_8$	0.005	$y_8y_9z_{10}z_{11}$	-0.008	$x_3x_6y_5z_3$	0.001	$y_0y_7z_1z_{10}$	-0.024
$x_8y_0z_0z_8$	-0.01	$x_2^2x_6z_5$	-0.013	$x_{10}y_0^2z_9$	-0.003	$y_0y_2^3$	-0.032
$z_{11}^2z_7z_9$	0.013	$x_0x_3y_6z_3$	-0.007	$x_1x_4x_6z_4$	-0.001	$y_{10}^2z_{10}z_8$	-0.048
$x_1x_{11}z_1z_8$	-0.046	$x_{10}x_{11}z_7^2$	-0.037	$x_0x_{10}x_7z_7$	-0.007	$y_0y_7z_1^2$	0.041
$x_{10}x_{11}y_8z_{11}$	-0.018	$x_8y_0y_{10}z_9$	-0.004	$x_2x_5x_6^2$	-0.006	$y_1y_4z_1z_6$	-0.003
$x_1x_7z_1z_7$	-1.465	$z_1^2z_5z_6$	-0.031	$x_6^2y_0z_4$	-0.005	$z_1z_3z_5z_6$	0.013
$x_2x_6z_2z_4$	0.008	$x_{11}x_7x_8y_9$	0.005	$x_3x_4y_5z_4$	-0.001	$x_0x_2z_1z_4$	0.012
$x_2^2z_5z_6$	0.1	z_{10}^4	2.008	$y_1y_2y_3y_4$	0.009	$x_7^2y_{11}z_9$	-0.003
$x_5^2y_3z_0$	0.041	$y_{10}z_{10}z_7z_9$	0.004	$x_3y_2z_3^2$	0.052	$x_6^2y_4z_5$	-0.037
$x_0x_7z_7^2$	0.326	$x_8x_9z_{11}z_9$	0.004	$x_0x_7z_1z_{11}$	-0.159	$y_{10}z_8^2z_9$	-0.0
$y_8y_9z_{10}^2$	0.075	$x_1^2z_3z_4$	0.003	$z_7^2z_8^2$	0.051	$x_1y_0y_2y_4$	0.097
$x_0x_4z_0z_3$	0.104	$z_0^2z_7^2$	0.06	$x_0x_{10}x_7x_9$	0.001	$x_3x_4z_5z_6$	-0.001
$x_1x_5y_1y_2$	0.005	$x_1x_7z_7z_8$	0.037	$x_0x_1z_0z_3$	-0.051	$x_1^2y_0y_3$	-0.093
$y_1^2y_5y_6$	-0.002	$x_2z_1^2z_5$	-0.003	$x_0^2z_6^2$	-0.515	$x_2x_6z_0z_2$	-0.15
$x_0x_{11}y_{10}z_9$	0.002	$y_7^2z_0^2$	0.017	$y_{11}z_{11}z_9^2$	-0.022	$x_7x_9z_{10}z_7$	-0.0
$x_2y_4z_5z_6$	-0.02	$y_{10}z_1z_{11}z_9$	0.021	$x_7x_8z_7^2$	0.01	$x_9y_{11}z_0z_8$	-0.003
$x_0x_6z_6^2$	0.959	$y_1y_5z_4^2$	0.002	$x_1x_6z_4z_6$	-0.007	$x_1^2x_2^2$	0.094
$x_3x_4z_4z_6$	-0.011	$x_2^2x_5x_6$	0.003	$y_1z_4^2z_6$	0.001	$x_1y_{10}y_7z_1$	-0.037
$x_7y_1z_7z_8$	0.035	$x_2y_2^2z_5$	0.054	$x_1^2x_4z_6$	0.002	$x_0^2y_4z_5$	0.06
$x_6^2z_0z_4$	-0.011	$x_4y_5z_1z_3$	0.002	$x_7y_1y_{11}z_8$	-0.012	$y_4y_5z_1z_2$	-0.003
$y_{10}z_{10}^2z_8$	-0.012	$x_5x_6z_0z_2$	0.007	$x_0x_1z_1^2$	0.58	$x_3x_4z_1z_3$	-0.001
$x_0^2x_1x_4$	0.015	$x_1^3x_2$	0.082	$x_7^2z_0z_7$	-0.001	$x_1x_7z_0z_7$	-0.036
$x_2y_1z_4^2$	-0.02	$x_4y_1y_5z_3$	-0.004	$x_{11}x_7^2z_1$	-0.023	$x_{10}y_7y_8z_{11}$	0.001
$y_8y_9z_{10}z_8$	0.024	$y_2^2z_2z_5$	0.031	$y_7^2z_0z_1$	-0.044		

Appendix E

Clebsh-Gordan Coefficients

The Clebsch-Gordan Coefficients for the terms derived for PbTe and Graphene are listed in the tables below.

Table E.1: Clebsch-Gordan Coefficients for 3rd order terms of graphene

Term Index	Clebsh-Gordan Coefficients
1	$\Theta^{111}_{E_{2g}B_{1u}E_{1u}} = 0.58, \Theta^{112}_{E_{2g}B_{1u}E_{1u}} = 11.702, \Theta^{211}_{E_{2g}B_{1u}E_{1u}} = 11.928, \Theta^{212}_{E_{2g}B_{1u}E_{1u}} = -0.544, \Theta^{311}_{E_{2g}B_{1u}E_{1u}} = -0.164, \Theta^{312}_{E_{2g}B_{1u}E_{1u}} = -2.239, \Theta^{411}_{E_{2g}B_{1u}E_{1u}} = 0.705, \Theta^{412}_{E_{2g}B_{1u}E_{1u}} = -0.946$
2	$\Theta^{112}_{A_{1g}E_{2g}E_{2g}} = 1.493, \Theta^{113}_{A_{1g}E_{2g}E_{2g}} = 0.108, \Theta^{114}_{A_{1g}E_{2g}E_{2g}} = 11.81, \Theta^{122}_{A_{1g}E_{2g}E_{2g}} = -0.853, \Theta^{123}_{A_{1g}E_{2g}E_{2g}} = 11.686, \Theta^{124}_{A_{1g}E_{2g}E_{2g}} = 0.108, \Theta^{133}_{A_{1g}E_{2g}E_{2g}} = 0.853, \Theta^{134}_{A_{1g}E_{2g}E_{2g}} = -1.493$
3	$\Theta^{111}_{E_{2g}E_{1u}E_{1u}} = -0.191, \Theta^{112}_{E_{2g}E_{1u}E_{1u}} = -0.705, \Theta^{122}_{E_{2g}E_{1u}E_{1u}} = 0.191, \Theta^{211}_{E_{2g}E_{1u}E_{1u}} = 0.423, \Theta^{212}_{E_{2g}E_{1u}E_{1u}} = -0.218, \Theta^{222}_{E_{2g}E_{1u}E_{1u}} = -0.423, \Theta^{311}_{E_{2g}E_{1u}E_{1u}} = -0.707, \Theta^{312}_{E_{2g}E_{1u}E_{1u}} = 0.32, \Theta^{322}_{E_{2g}E_{1u}E_{1u}} = 0.707, \Theta^{411}_{E_{2g}E_{1u}E_{1u}} = 0.122, \Theta^{412}_{E_{2g}E_{1u}E_{1u}} = 1.508, \Theta^{422}_{E_{2g}E_{1u}E_{1u}} = -0.122$
4	$\Theta^{111}_{E_{2g}B_{1u}E_{1u}} = -0.172, \Theta^{112}_{E_{2g}B_{1u}E_{1u}} = -0.58, \Theta^{211}_{E_{2g}B_{1u}E_{1u}} = -0.544, \Theta^{212}_{E_{2g}B_{1u}E_{1u}} = 0.072, \Theta^{311}_{E_{2g}B_{1u}E_{1u}} = -0.73, \Theta^{312}_{E_{2g}B_{1u}E_{1u}} = 0.164, \Theta^{411}_{E_{2g}B_{1u}E_{1u}} = -0.084, \Theta^{412}_{E_{2g}B_{1u}E_{1u}} = -0.705$
5	$\Theta^{111}_{A_{1g}E_{2g}E_{2g}} = 11.173, \Theta^{112}_{A_{1g}E_{2g}E_{2g}} = 0.299, \Theta^{113}_{A_{1g}E_{2g}E_{2g}} = -4.125, \Theta^{122}_{A_{1g}E_{2g}E_{2g}} = 11.47, \Theta^{123}_{A_{1g}E_{2g}E_{2g}} = 1.545, \Theta^{124}_{A_{1g}E_{2g}E_{2g}} = 1.42, \Theta^{133}_{A_{1g}E_{2g}E_{2g}} = 0.883, \Theta^{134}_{A_{1g}E_{2g}E_{2g}} = 0.103, \Theta^{144}_{A_{1g}E_{2g}E_{2g}} = 0.474$
6	$\Theta^{111}_{E_{2g}E_{1u}E_{1u}} = 0.812, \Theta^{112}_{E_{2g}E_{1u}E_{1u}} = 11.499, \Theta^{122}_{E_{2g}E_{1u}E_{1u}} = -0.812, \Theta^{211}_{E_{2g}E_{1u}E_{1u}} = -5.85, \Theta^{212}_{E_{2g}E_{1u}E_{1u}} = 1.719, \Theta^{222}_{E_{2g}E_{1u}E_{1u}} = 5.85, \Theta^{311}_{E_{2g}E_{1u}E_{1u}} = -0.202, \Theta^{312}_{E_{2g}E_{1u}E_{1u}} = -2.192, \Theta^{322}_{E_{2g}E_{1u}E_{1u}} = 0.202, \Theta^{411}_{E_{2g}E_{1u}E_{1u}} = -0.423, \Theta^{412}_{E_{2g}E_{1u}E_{1u}} = -0.644, \Theta^{422}_{E_{2g}E_{1u}E_{1u}} = 0.423$
7	$\Theta^{111}_{E_{2g}B_{2u}E_{1u}} = -0.564, \Theta^{112}_{E_{2g}B_{2u}E_{1u}} = 2.257, \Theta^{211}_{E_{2g}B_{2u}E_{1u}} = 0.73, \Theta^{212}_{E_{2g}B_{2u}E_{1u}} = -0.164, \Theta^{311}_{E_{2g}B_{2u}E_{1u}} = 0.928, \Theta^{312}_{E_{2g}B_{2u}E_{1u}} = 11.5, \Theta^{411}_{E_{2g}B_{2u}E_{1u}} = -11.674, \Theta^{412}_{E_{2g}B_{2u}E_{1u}} = 0.795$

8	$\Theta^{111}_{A_{1g}B_{2u}B_{2u}} = 24.0$
9	$\Theta^{111}_{A_{1g}E_{2g}E_{2g}} = 0.15, \Theta^{112}_{A_{1g}E_{2g}E_{2g}} = 0.197, \Theta^{113}_{A_{1g}E_{2g}E_{2g}} = -0.106, \Theta^{114}_{A_{1g}E_{2g}E_{2g}} = 1.493, \Theta^{122}_{A_{1g}E_{2g}E_{2g}} = 0.05, \Theta^{123}_{A_{1g}E_{2g}E_{2g}} = 1.522, \Theta^{124}_{A_{1g}E_{2g}E_{2g}} = 0.055, \Theta^{133}_{A_{1g}E_{2g}E_{2g}} = -0.04, \Theta^{134}_{A_{1g}E_{2g}E_{2g}} = -0.186, \Theta^{144}_{A_{1g}E_{2g}E_{2g}} = -0.16$
10	$\Theta^{111}_{E_{2g}E_{2g}E_{2g}} = -0.384, \Theta^{112}_{E_{2g}E_{2g}E_{2g}} = -0.322, \Theta^{113}_{E_{2g}E_{2g}E_{2g}} = -1.794, \Theta^{114}_{E_{2g}E_{2g}E_{2g}} = -0.108, \Theta^{122}_{E_{2g}E_{2g}E_{2g}} = 0.654, \Theta^{123}_{E_{2g}E_{2g}E_{2g}} = 0.179, \Theta^{124}_{E_{2g}E_{2g}E_{2g}} = -4.01, \Theta^{133}_{E_{2g}E_{2g}E_{2g}} = 1.379, \Theta^{134}_{E_{2g}E_{2g}E_{2g}} = -0.668, \Theta^{144}_{E_{2g}E_{2g}E_{2g}} = -0.882, \Theta^{222}_{E_{2g}E_{2g}E_{2g}} = 0.012, \Theta^{223}_{E_{2g}E_{2g}E_{2g}} = 2.019, \Theta^{224}_{E_{2g}E_{2g}E_{2g}} = -0.049, \Theta^{233}_{E_{2g}E_{2g}E_{2g}} = 0.267, \Theta^{234}_{E_{2g}E_{2g}E_{2g}} = 1.462, \Theta^{244}_{E_{2g}E_{2g}E_{2g}} = 0.02, \Theta^{333}_{E_{2g}E_{2g}E_{2g}} = 0.971, \Theta^{334}_{E_{2g}E_{2g}E_{2g}} = 0.197, \Theta^{344}_{E_{2g}E_{2g}E_{2g}} = -3.137, \Theta^{444}_{E_{2g}E_{2g}E_{2g}} = -0.013$
11	$\Theta^{111}_{E_{2g}B_{2u}E_{1u}} = -2.257, \Theta^{112}_{E_{2g}B_{2u}E_{1u}} = 0.298, \Theta^{211}_{E_{2g}B_{2u}E_{1u}} = 0.164, \Theta^{212}_{E_{2g}B_{2u}E_{1u}} = 2.239, \Theta^{311}_{E_{2g}B_{2u}E_{1u}} = 0.5, \Theta^{312}_{E_{2g}B_{2u}E_{1u}} = 0.928, \Theta^{411}_{E_{2g}B_{2u}E_{1u}} = -0.795, \Theta^{412}_{E_{2g}B_{2u}E_{1u}} = 0.199$
12	$\Theta^{111}_{E_{2g}E_{2g}E_{2g}} = 0.129, \Theta^{112}_{E_{2g}E_{2g}E_{2g}} = -0.039, \Theta^{113}_{E_{2g}E_{2g}E_{2g}} = 0.536, \Theta^{122}_{E_{2g}E_{2g}E_{2g}} = -0.235, \Theta^{123}_{E_{2g}E_{2g}E_{2g}} = 0.094, \Theta^{124}_{E_{2g}E_{2g}E_{2g}} = 1.354, \Theta^{133}_{E_{2g}E_{2g}E_{2g}} = -0.882, \Theta^{134}_{E_{2g}E_{2g}E_{2g}} = 0.098, \Theta^{144}_{E_{2g}E_{2g}E_{2g}} = 0.731, \Theta^{222}_{E_{2g}E_{2g}E_{2g}} = 0.051, \Theta^{223}_{E_{2g}E_{2g}E_{2g}} = -0.704, \Theta^{224}_{E_{2g}E_{2g}E_{2g}} = 0.058, \Theta^{233}_{E_{2g}E_{2g}E_{2g}} = 0.125, \Theta^{234}_{E_{2g}E_{2g}E_{2g}} = -0.791, \Theta^{244}_{E_{2g}E_{2g}E_{2g}} = -0.238, \Theta^{333}_{E_{2g}E_{2g}E_{2g}} = -1.039, \Theta^{334}_{E_{2g}E_{2g}E_{2g}} = -0.058, \Theta^{344}_{E_{2g}E_{2g}E_{2g}} = 3.283$
13	$\Theta^{111}_{E_{2g}E_{2g}E_{2g}} = 0.005, \Theta^{112}_{E_{2g}E_{2g}E_{2g}} = -0.424, \Theta^{113}_{E_{2g}E_{2g}E_{2g}} = 0.025, \Theta^{114}_{E_{2g}E_{2g}E_{2g}} = 2.167, \Theta^{122}_{E_{2g}E_{2g}E_{2g}} = 0.203, \Theta^{123}_{E_{2g}E_{2g}E_{2g}} = -2.863, \Theta^{124}_{E_{2g}E_{2g}E_{2g}} = -0.727, \Theta^{133}_{E_{2g}E_{2g}E_{2g}} = 0.02, \Theta^{134}_{E_{2g}E_{2g}E_{2g}} = 10.769, \Theta^{144}_{E_{2g}E_{2g}E_{2g}} = -0.238, \Theta^{222}_{E_{2g}E_{2g}E_{2g}} = 0.02, \Theta^{223}_{E_{2g}E_{2g}E_{2g}} = 0.796, \Theta^{224}_{E_{2g}E_{2g}E_{2g}} = -0.766, \Theta^{233}_{E_{2g}E_{2g}E_{2g}} = -5.526, \Theta^{234}_{E_{2g}E_{2g}E_{2g}} = 0.413, \Theta^{244}_{E_{2g}E_{2g}E_{2g}} = 5.889, \Theta^{333}_{E_{2g}E_{2g}E_{2g}} = 0.001, \Theta^{334}_{E_{2g}E_{2g}E_{2g}} = -2.529, \Theta^{344}_{E_{2g}E_{2g}E_{2g}} = -0.822, \Theta^{444}_{E_{2g}E_{2g}E_{2g}} = 0.376$
14	$\Theta^{111}_{E_{2g}E_{2g}E_{2g}} = 0.598, \Theta^{112}_{E_{2g}E_{2g}E_{2g}} = -0.209, \Theta^{113}_{E_{2g}E_{2g}E_{2g}} = 2.873, \Theta^{122}_{E_{2g}E_{2g}E_{2g}} = -1.03, \Theta^{123}_{E_{2g}E_{2g}E_{2g}} = 0.018, \Theta^{124}_{E_{2g}E_{2g}E_{2g}} = 6.297, \Theta^{133}_{E_{2g}E_{2g}E_{2g}} = -1.151, \Theta^{134}_{E_{2g}E_{2g}E_{2g}} = 0.457, \Theta^{144}_{E_{2g}E_{2g}E_{2g}} = 0.386, \Theta^{222}_{E_{2g}E_{2g}E_{2g}} = 0.225, \Theta^{223}_{E_{2g}E_{2g}E_{2g}} = -3.069, \Theta^{224}_{E_{2g}E_{2g}E_{2g}} = 0.117, \Theta^{233}_{E_{2g}E_{2g}E_{2g}} = -0.483, \Theta^{234}_{E_{2g}E_{2g}E_{2g}} = -1.609, \Theta^{244}_{E_{2g}E_{2g}E_{2g}} = 0.015, \Theta^{333}_{E_{2g}E_{2g}E_{2g}} = 0.136, \Theta^{334}_{E_{2g}E_{2g}E_{2g}} = -0.117, \Theta^{344}_{E_{2g}E_{2g}E_{2g}} = -0.211$
15	$\Theta^{111}_{A_{1g}A_{1g}A_{1g}} = 24.0$
16	$\Theta^{111}_{A_{2g}B_{1u}B_{2u}} = 24.0$

17	$\Theta^{111}_{A_{2g}E_{2g}E_{2g}} = -0.16, \Theta^{112}_{A_{2g}E_{2g}E_{2g}} = 0.058, \Theta^{113}_{A_{2g}E_{2g}E_{2g}} = -0.798, \Theta^{122}_{A_{2g}E_{2g}E_{2g}} = -0.054, \Theta^{123}_{A_{2g}E_{2g}E_{2g}} = -0.031, \Theta^{124}_{A_{2g}E_{2g}E_{2g}} = 0.852, \Theta^{133}_{A_{2g}E_{2g}E_{2g}} = 0.159, \Theta^{134}_{A_{2g}E_{2g}E_{2g}} = 0.062, \Theta^{144}_{A_{2g}E_{2g}E_{2g}} = 0.055$
18	$\Theta^{111}_{A_{1g}A_{2g}A_{2g}} = 24.0$
19	$\Theta^{111}_{A_{1g}E_{1u}E_{1u}} = 12.0, \Theta^{122}_{A_{1g}E_{1u}E_{1u}} = 12.0$
20	$\Theta^{111}_{A_{1g}B_{1u}B_{1u}} = 24.0$

Table E.2: Clebsch-Gordan Coefficients for 4th order terms of graphene

Term Index	Clebsh-Gordan Coefficients
1	$\Theta^{1112}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.044, \Theta^{1113}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.003, \Theta^{1114}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.35, \Theta^{1122}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.055, \Theta^{1123}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.755, \Theta^{1124}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.233, \Theta^{1133}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.055, \Theta^{1134}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 3.208, \Theta^{1222}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.032, \Theta^{1223}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.621, \Theta^{1224}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.027, \Theta^{1233}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 4.26, \Theta^{1234}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -1.179, \Theta^{1244}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.009, \Theta^{1333}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.312, \Theta^{1334}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 8.052, \Theta^{1344}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.001, \Theta^{1444}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 8.785, \Theta^{2222}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.008, \Theta^{2223}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.203, \Theta^{2224}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.082, \Theta^{2233}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -1.808, \Theta^{2234}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -1.128, \Theta^{2244}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.645, \Theta^{2333}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 8.287, \Theta^{2334}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.07, \Theta^{2344}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 8.834, \Theta^{2444}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.081, \Theta^{3333}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.611, \Theta^{3334}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -1.076, \Theta^{3344}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.645, \Theta^{3444}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -1.111$
2	$\Theta^{1111}_{E_{2g}E_{2g}B_{2u}E_{1u}} = -0.113, \Theta^{1112}_{E_{2g}E_{2g}B_{2u}E_{1u}} = -0.346, \Theta^{1211}_{E_{2g}E_{2g}B_{2u}E_{1u}} = 0.757, \Theta^{1212}_{E_{2g}E_{2g}B_{2u}E_{1u}} = -0.193, \Theta^{1311}_{E_{2g}E_{2g}B_{2u}E_{1u}} = -0.381, \Theta^{1312}_{E_{2g}E_{2g}B_{2u}E_{1u}} = 0.309, \Theta^{1411}_{E_{2g}E_{2g}B_{2u}E_{1u}} = 0.232, \Theta^{1412}_{E_{2g}E_{2g}B_{2u}E_{1u}} = 0.459, \Theta^{2211}_{E_{2g}E_{2g}B_{2u}E_{1u}} = 0.072, \Theta^{2212}_{E_{2g}E_{2g}B_{2u}E_{1u}} = 0.408, \Theta^{2311}_{E_{2g}E_{2g}B_{2u}E_{1u}} = -0.231, \Theta^{2312}_{E_{2g}E_{2g}B_{2u}E_{1u}} = -0.455, \Theta^{2411}_{E_{2g}E_{2g}B_{2u}E_{1u}} = -0.533, \Theta^{2412}_{E_{2g}E_{2g}B_{2u}E_{1u}} = 0.144, \Theta^{3311}_{E_{2g}E_{2g}B_{2u}E_{1u}} = 0.098, \Theta^{3312}_{E_{2g}E_{2g}B_{2u}E_{1u}} = 0.341, \Theta^{3411}_{E_{2g}E_{2g}B_{2u}E_{1u}} = 0.746, \Theta^{3412}_{E_{2g}E_{2g}B_{2u}E_{1u}} = -0.163, \Theta^{4411}_{E_{2g}E_{2g}B_{2u}E_{1u}} = -0.057, \Theta^{4412}_{E_{2g}E_{2g}B_{2u}E_{1u}} = -0.403$
3	$\Theta^{1111}_{A_{2g}E_{2g}E_{2g}E_{2g}} = 0.161, \Theta^{1112}_{A_{2g}E_{2g}E_{2g}E_{2g}} = -0.931, \Theta^{1113}_{A_{2g}E_{2g}E_{2g}E_{2g}} = -0.112, \Theta^{1114}_{A_{2g}E_{2g}E_{2g}E_{2g}} = 2.002, \Theta^{1122}_{A_{2g}E_{2g}E_{2g}E_{2g}} = -0.2, \Theta^{1123}_{A_{2g}E_{2g}E_{2g}E_{2g}} = -4.0, \Theta^{1124}_{A_{2g}E_{2g}E_{2g}E_{2g}} = 0.109, \Theta^{1133}_{A_{2g}E_{2g}E_{2g}E_{2g}} = -0.158, \Theta^{1134}_{A_{2g}E_{2g}E_{2g}E_{2g}} = -1.464, \Theta^{1144}_{A_{2g}E_{2g}E_{2g}E_{2g}} = -0.125, \Theta^{1222}_{A_{2g}E_{2g}E_{2g}E_{2g}} = 0.136, \Theta^{1223}_{A_{2g}E_{2g}E_{2g}E_{2g}} = -0.019, \Theta^{1224}_{A_{2g}E_{2g}E_{2g}E_{2g}} = -2.151, \Theta^{1233}_{A_{2g}E_{2g}E_{2g}E_{2g}} = 0.87, \Theta^{1234}_{A_{2g}E_{2g}E_{2g}E_{2g}} = 0.081, \Theta^{1244}_{A_{2g}E_{2g}E_{2g}E_{2g}} = -0.348, \Theta^{1333}_{A_{2g}E_{2g}E_{2g}E_{2g}} = 0.039, \Theta^{1334}_{A_{2g}E_{2g}E_{2g}E_{2g}} = -0.908, \Theta^{1344}_{A_{2g}E_{2g}E_{2g}E_{2g}} = 0.016, \Theta^{1444}_{A_{2g}E_{2g}E_{2g}E_{2g}} = 0.352$

4	$\Theta^{1111}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 8.574, \Theta^{1112}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -0.557, \Theta^{1122}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 2.895, \Theta^{1211}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -0.497, \Theta^{1212}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -11.58, \Theta^{1222}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.598, \Theta^{1311}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -3.267, \Theta^{1312}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.301, \Theta^{1322}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -1.11, \Theta^{1411}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -1.347, \Theta^{1412}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -0.627, \Theta^{1422}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -0.358, \Theta^{2211}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 3.001, \Theta^{2212}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.537, \Theta^{2222}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 8.905, \Theta^{2311}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.121, \Theta^{2312}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 2.206, \Theta^{2322}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -0.175, \Theta^{2411}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.418, \Theta^{2412}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 1.003, \Theta^{2422}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 1.068, \Theta^{3311}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.348, \Theta^{3312}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -0.04, \Theta^{3322}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.119, \Theta^{3411}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.263, \Theta^{3412}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.16, \Theta^{3422}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.062, \Theta^{4411}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.077, \Theta^{4412}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.06, \Theta^{4422}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.081$
5	$\Theta^{1111}_{A_{2g}A_{2g}E_{1u}E_{1u}} = 12.0, \Theta^{1122}_{A_{2g}A_{2g}E_{1u}E_{1u}} = 12.0$
6	$\Theta^{1111}_{A_{1g}A_{1g}E_{2g}E_{2g}} = 0.052, \Theta^{1112}_{A_{1g}A_{1g}E_{2g}E_{2g}} = -0.186, \Theta^{1113}_{A_{1g}A_{1g}E_{2g}E_{2g}} = -0.055, \Theta^{1114}_{A_{1g}A_{1g}E_{2g}E_{2g}} = -1.493, \Theta^{1122}_{A_{1g}A_{1g}E_{2g}E_{2g}} = 0.162, \Theta^{1123}_{A_{1g}A_{1g}E_{2g}E_{2g}} = -1.462, \Theta^{1124}_{A_{1g}A_{1g}E_{2g}E_{2g}} = 0.0, \Theta^{1133}_{A_{1g}A_{1g}E_{2g}E_{2g}} = -0.159, \Theta^{1134}_{A_{1g}A_{1g}E_{2g}E_{2g}} = 0.19, \Theta^{1144}_{A_{1g}A_{1g}E_{2g}E_{2g}} = -0.055$
7	$\Theta^{1111}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -1.334, \Theta^{1112}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.19, \Theta^{1113}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 2.744, \Theta^{1114}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.076, \Theta^{1122}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -2.923, \Theta^{1123}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.84, \Theta^{1124}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -1.711, \Theta^{1133}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 3.334, \Theta^{1134}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.162, \Theta^{1144}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 1.404, \Theta^{1222}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.143, \Theta^{1223}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 2.068, \Theta^{1224}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.469, \Theta^{1233}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.606, \Theta^{1234}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -5.338, \Theta^{1244}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.074, \Theta^{1333}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -1.493, \Theta^{1334}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.381, \Theta^{1344}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.885, \Theta^{1444}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.003, \Theta^{2222}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -1.557, \Theta^{2223}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.562, \Theta^{2224}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.982, \Theta^{2233}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 1.231, \Theta^{2234}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.401, \Theta^{2244}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 4.467, \Theta^{2333}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.129, \Theta^{2334}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 1.254, \Theta^{2344}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.614, \Theta^{2444}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.57, \Theta^{3333}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.218, \Theta^{3334}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.092, \Theta^{3344}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.271, \Theta^{3444}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.041, \Theta^{4444}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.078$

8	$\Theta^{1111}_{A_{2g}E_{2g}E_{2g}E_{2g}} = -0.958, \Theta^{1112}_{A_{2g}E_{2g}E_{2g}E_{2g}} = -0.018, \Theta^{1113}_{A_{2g}E_{2g}E_{2g}E_{2g}} = 1.364, \Theta^{1114}_{A_{2g}E_{2g}E_{2g}E_{2g}} = -0.176, \Theta^{1122}_{A_{2g}E_{2g}E_{2g}E_{2g}} = 3.107, \Theta^{1123}_{A_{2g}E_{2g}E_{2g}E_{2g}} = 0.539, \Theta^{1124}_{A_{2g}E_{2g}E_{2g}E_{2g}} = 1.471, \Theta^{1133}_{A_{2g}E_{2g}E_{2g}E_{2g}} = 1.794, \Theta^{1134}_{A_{2g}E_{2g}E_{2g}E_{2g}} = 0.198, \Theta^{1144}_{A_{2g}E_{2g}E_{2g}E_{2g}} = -2.029, \Theta^{1222}_{A_{2g}E_{2g}E_{2g}E_{2g}} = 0.051, \Theta^{1223}_{A_{2g}E_{2g}E_{2g}E_{2g}} = -0.865, \Theta^{1224}_{A_{2g}E_{2g}E_{2g}E_{2g}} = -0.108, \Theta^{1233}_{A_{2g}E_{2g}E_{2g}E_{2g}} = -0.112, \Theta^{1234}_{A_{2g}E_{2g}E_{2g}E_{2g}} = 4.025, \Theta^{1244}_{A_{2g}E_{2g}E_{2g}E_{2g}} = -0.025, \Theta^{1333}_{A_{2g}E_{2g}E_{2g}E_{2g}} = -0.389, \Theta^{1334}_{A_{2g}E_{2g}E_{2g}E_{2g}} = 0.279, \Theta^{1344}_{A_{2g}E_{2g}E_{2g}E_{2g}} = 0.669, \Theta^{1444}_{A_{2g}E_{2g}E_{2g}E_{2g}} = 0.002$
9	$\Theta^{1111}_{A_{1g}E_{2g}E_{2g}E_{2g}} = -0.07, \Theta^{1112}_{A_{1g}E_{2g}E_{2g}E_{2g}} = 0.025, \Theta^{1113}_{A_{1g}E_{2g}E_{2g}E_{2g}} = -0.764, \Theta^{1114}_{A_{1g}E_{2g}E_{2g}E_{2g}} = 0.157, \Theta^{1122}_{A_{1g}E_{2g}E_{2g}E_{2g}} = 0.065, \Theta^{1123}_{A_{1g}E_{2g}E_{2g}E_{2g}} = 0.258, \Theta^{1124}_{A_{1g}E_{2g}E_{2g}E_{2g}} = -0.803, \Theta^{1133}_{A_{1g}E_{2g}E_{2g}E_{2g}} = -3.137, \Theta^{1134}_{A_{1g}E_{2g}E_{2g}E_{2g}} = 0.727, \Theta^{1144}_{A_{1g}E_{2g}E_{2g}E_{2g}} = 3.283, \Theta^{1222}_{A_{1g}E_{2g}E_{2g}E_{2g}} = -0.013, \Theta^{1223}_{A_{1g}E_{2g}E_{2g}E_{2g}} = 0.199, \Theta^{1224}_{A_{1g}E_{2g}E_{2g}E_{2g}} = 0.098, \Theta^{1233}_{A_{1g}E_{2g}E_{2g}E_{2g}} = 0.837, \Theta^{1234}_{A_{1g}E_{2g}E_{2g}E_{2g}} = -2.077, \Theta^{1244}_{A_{1g}E_{2g}E_{2g}E_{2g}} = -0.822, \Theta^{1333}_{A_{1g}E_{2g}E_{2g}E_{2g}} = -5.532, \Theta^{1334}_{A_{1g}E_{2g}E_{2g}E_{2g}} = -0.337, \Theta^{1344}_{A_{1g}E_{2g}E_{2g}E_{2g}} = 17.16, \Theta^{1444}_{A_{1g}E_{2g}E_{2g}E_{2g}} = 0.027$
10	$\Theta^{1111}_{A_{2g}E_{2g}E_{1u}E_{1u}} = -5.695, \Theta^{1112}_{A_{2g}E_{2g}E_{1u}E_{1u}} = 1.412, \Theta^{1122}_{A_{2g}E_{2g}E_{1u}E_{1u}} = 5.695, \Theta^{1211}_{A_{2g}E_{2g}E_{1u}E_{1u}} = -0.812, \Theta^{1212}_{A_{2g}E_{2g}E_{1u}E_{1u}} = -11.499, \Theta^{1222}_{A_{2g}E_{2g}E_{1u}E_{1u}} = 0.812, \Theta^{1311}_{A_{2g}E_{2g}E_{1u}E_{1u}} = 1.021, \Theta^{1312}_{A_{2g}E_{2g}E_{1u}E_{1u}} = -1.401, \Theta^{1322}_{A_{2g}E_{2g}E_{1u}E_{1u}} = -1.021, \Theta^{1411}_{A_{2g}E_{2g}E_{1u}E_{1u}} = -0.191, \Theta^{1412}_{A_{2g}E_{2g}E_{1u}E_{1u}} = -0.705, \Theta^{1422}_{A_{2g}E_{2g}E_{1u}E_{1u}} = 0.191$
11	$\Theta^{1111}_{A_{2g}E_{2g}E_{2g}E_{2g}} = 0.07, \Theta^{1112}_{A_{2g}E_{2g}E_{2g}E_{2g}} = 1.122, \Theta^{1113}_{A_{2g}E_{2g}E_{2g}E_{2g}} = -0.018, \Theta^{1114}_{A_{2g}E_{2g}E_{2g}E_{2g}} = -2.428, \Theta^{1122}_{A_{2g}E_{2g}E_{2g}E_{2g}} = -0.569, \Theta^{1123}_{A_{2g}E_{2g}E_{2g}E_{2g}} = 4.668, \Theta^{1124}_{A_{2g}E_{2g}E_{2g}E_{2g}} = -0.198, \Theta^{1133}_{A_{2g}E_{2g}E_{2g}E_{2g}} = 0.213, \Theta^{1134}_{A_{2g}E_{2g}E_{2g}E_{2g}} = 1.239, \Theta^{1144}_{A_{2g}E_{2g}E_{2g}E_{2g}} = 0.147, \Theta^{1222}_{A_{2g}E_{2g}E_{2g}E_{2g}} = -0.173, \Theta^{1223}_{A_{2g}E_{2g}E_{2g}E_{2g}} = 0.164, \Theta^{1224}_{A_{2g}E_{2g}E_{2g}E_{2g}} = 2.556, \Theta^{1233}_{A_{2g}E_{2g}E_{2g}E_{2g}} = -0.931, \Theta^{1234}_{A_{2g}E_{2g}E_{2g}E_{2g}} = 0.106, \Theta^{1244}_{A_{2g}E_{2g}E_{2g}E_{2g}} = 0.329, \Theta^{1333}_{A_{2g}E_{2g}E_{2g}E_{2g}} = -0.041, \Theta^{1334}_{A_{2g}E_{2g}E_{2g}E_{2g}} = -0.2, \Theta^{1344}_{A_{2g}E_{2g}E_{2g}E_{2g}} = -0.025, \Theta^{1444}_{A_{2g}E_{2g}E_{2g}E_{2g}} = 0.024$

12	$\Theta^{1111}_{A_{1g}E_{2g}E_{2g}E_{2g}} = -0.07, \Theta^{1112}_{A_{1g}E_{2g}E_{2g}E_{2g}} = 16.627, \Theta^{1113}_{A_{1g}E_{2g}E_{2g}E_{2g}} = 0.871, \Theta^{1114}_{A_{1g}E_{2g}E_{2g}E_{2g}} = 0.936, \Theta^{1122}_{A_{1g}E_{2g}E_{2g}E_{2g}} = 0.569, \Theta^{1123}_{A_{1g}E_{2g}E_{2g}E_{2g}} = -6.161, \Theta^{1124}_{A_{1g}E_{2g}E_{2g}E_{2g}} = -0.655, \Theta^{1133}_{A_{1g}E_{2g}E_{2g}E_{2g}} = -0.322, \Theta^{1134}_{A_{1g}E_{2g}E_{2g}E_{2g}} = -1.111, \Theta^{1144}_{A_{1g}E_{2g}E_{2g}E_{2g}} = -0.039, \Theta^{1222}_{A_{1g}E_{2g}E_{2g}E_{2g}} = -5.701, \Theta^{1223}_{A_{1g}E_{2g}E_{2g}E_{2g}} = -1.017, \Theta^{1224}_{A_{1g}E_{2g}E_{2g}E_{2g}} = -1.063, \Theta^{1233}_{A_{1g}E_{2g}E_{2g}E_{2g}} = 0.9, \Theta^{1234}_{A_{1g}E_{2g}E_{2g}E_{2g}} = 0.002, \Theta^{1244}_{A_{1g}E_{2g}E_{2g}E_{2g}} = -0.424, \Theta^{1333}_{A_{1g}E_{2g}E_{2g}E_{2g}} = 0.041, \Theta^{1334}_{A_{1g}E_{2g}E_{2g}E_{2g}} = 0.2, \Theta^{1344}_{A_{1g}E_{2g}E_{2g}E_{2g}} = 0.025, \Theta^{1444}_{A_{1g}E_{2g}E_{2g}E_{2g}} = -0.024$
13	$\Theta^{1111}_{A_{1g}E_{2g}E_{1u}E_{1u}} = -0.305, \Theta^{1112}_{A_{1g}E_{2g}E_{1u}E_{1u}} = -1.412, \Theta^{1122}_{A_{1g}E_{2g}E_{1u}E_{1u}} = 0.305, \Theta^{1211}_{A_{1g}E_{2g}E_{1u}E_{1u}} = 0.812, \Theta^{1212}_{A_{1g}E_{2g}E_{1u}E_{1u}} = -0.375, \Theta^{1222}_{A_{1g}E_{2g}E_{1u}E_{1u}} = -0.812, \Theta^{1311}_{A_{1g}E_{2g}E_{1u}E_{1u}} = -1.021, \Theta^{1312}_{A_{1g}E_{2g}E_{1u}E_{1u}} = 0.539, \Theta^{1322}_{A_{1g}E_{2g}E_{1u}E_{1u}} = 1.021, \Theta^{1411}_{A_{1g}E_{2g}E_{1u}E_{1u}} = 0.191, \Theta^{1412}_{A_{1g}E_{2g}E_{1u}E_{1u}} = 2.214, \Theta^{1422}_{A_{1g}E_{2g}E_{1u}E_{1u}} = -0.191$
14	$\Theta^{1111}_{E_{2g}E_{2g}B_{1u}E_{1u}} = 0.113, \Theta^{1112}_{E_{2g}E_{2g}B_{1u}E_{1u}} = 1.093, \Theta^{1211}_{E_{2g}E_{2g}B_{1u}E_{1u}} = -1.512, \Theta^{1212}_{E_{2g}E_{2g}B_{1u}E_{1u}} = -0.234, \Theta^{1311}_{E_{2g}E_{2g}B_{1u}E_{1u}} = 0.381, \Theta^{1312}_{E_{2g}E_{2g}B_{1u}E_{1u}} = 5.471, \Theta^{1411}_{E_{2g}E_{2g}B_{1u}E_{1u}} = 5.705, \Theta^{1412}_{E_{2g}E_{2g}B_{1u}E_{1u}} = -0.514, \Theta^{2211}_{E_{2g}E_{2g}B_{1u}E_{1u}} = 0.359, \Theta^{2212}_{E_{2g}E_{2g}B_{1u}E_{1u}} = -0.408, \Theta^{2311}_{E_{2g}E_{2g}B_{1u}E_{1u}} = -5.705, \Theta^{2312}_{E_{2g}E_{2g}B_{1u}E_{1u}} = 0.509, \Theta^{2411}_{E_{2g}E_{2g}B_{1u}E_{1u}} = 0.533, \Theta^{2412}_{E_{2g}E_{2g}B_{1u}E_{1u}} = 5.887, \Theta^{3311}_{E_{2g}E_{2g}B_{1u}E_{1u}} = -0.098, \Theta^{3312}_{E_{2g}E_{2g}B_{1u}E_{1u}} = -1.087, \Theta^{3411}_{E_{2g}E_{2g}B_{1u}E_{1u}} = -1.5, \Theta^{3412}_{E_{2g}E_{2g}B_{1u}E_{1u}} = -0.263, \Theta^{4411}_{E_{2g}E_{2g}B_{1u}E_{1u}} = -0.374, \Theta^{4412}_{E_{2g}E_{2g}B_{1u}E_{1u}} = 0.403$
15	$\Theta^{1111}_{A_{2g}E_{2g}E_{1u}E_{1u}} = 1.021, \Theta^{1112}_{A_{2g}E_{2g}E_{1u}E_{1u}} = -0.539, \Theta^{1122}_{A_{2g}E_{2g}E_{1u}E_{1u}} = -1.021, \Theta^{1211}_{A_{2g}E_{2g}E_{1u}E_{1u}} = 0.202, \Theta^{1212}_{A_{2g}E_{2g}E_{1u}E_{1u}} = 2.192, \Theta^{1222}_{A_{2g}E_{2g}E_{1u}E_{1u}} = -0.202, \Theta^{1311}_{A_{2g}E_{2g}E_{1u}E_{1u}} = -0.277, \Theta^{1312}_{A_{2g}E_{2g}E_{1u}E_{1u}} = -1.202, \Theta^{1322}_{A_{2g}E_{2g}E_{1u}E_{1u}} = 0.277, \Theta^{1411}_{A_{2g}E_{2g}E_{1u}E_{1u}} = -0.707, \Theta^{1412}_{A_{2g}E_{2g}E_{1u}E_{1u}} = 0.32, \Theta^{1422}_{A_{2g}E_{2g}E_{1u}E_{1u}} = 0.707$

16	$\Theta^{1111}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -0.071, \Theta^{1112}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 1.047, \Theta^{1122}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.071, \Theta^{1211}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.694, \Theta^{1212}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.005, \Theta^{1222}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -0.694, \Theta^{1311}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.402, \Theta^{1312}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 5.07, \Theta^{1322}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -0.402, \Theta^{1411}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -2.64, \Theta^{1412}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.66, \Theta^{1422}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 2.64, \Theta^{2211}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -0.075, \Theta^{2212}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -0.332, \Theta^{2222}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.075, \Theta^{2311}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 2.642, \Theta^{2312}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -0.67, \Theta^{2322}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -2.642, \Theta^{2411}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.308, \Theta^{2412}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 5.425, \Theta^{2422}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -0.308, \Theta^{3311}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.051, \Theta^{3312}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -1.045, \Theta^{3322}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -0.051, \Theta^{3411}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.691, \Theta^{3412}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -0.077, \Theta^{3422}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -0.691, \Theta^{4411}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.096, \Theta^{4412}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.329, \Theta^{4422}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -0.096$
17	$\Theta^{1111}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.353, \Theta^{1112}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -0.048, \Theta^{1122}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.122, \Theta^{1211}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -0.263, \Theta^{1212}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -0.159, \Theta^{1222}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -0.057, \Theta^{1311}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 3.279, \Theta^{1312}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -0.383, \Theta^{1322}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 1.127, \Theta^{1411}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.19, \Theta^{1412}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 2.202, \Theta^{1422}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -0.19, \Theta^{2211}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.077, \Theta^{2212}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.06, \Theta^{2222}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.081, \Theta^{2311}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -1.331, \Theta^{2312}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -0.606, \Theta^{2322}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -0.319, \Theta^{2411}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -0.444, \Theta^{2412}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -1.027, \Theta^{2422}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -1.072, \Theta^{3311}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 8.547, \Theta^{3312}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -0.76, \Theta^{3322}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 2.919, \Theta^{3411}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.7, \Theta^{3412}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 11.48, \Theta^{3422}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -0.81, \Theta^{4411}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 3.024, \Theta^{4412}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.748, \Theta^{4422}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 8.878$
18	$\Theta^{1111}_{A_{1g}A_{2g}E_{2g}E_{2g}} = -0.821, \Theta^{1112}_{A_{1g}A_{2g}E_{2g}E_{2g}} = 0.297, \Theta^{1113}_{A_{1g}A_{2g}E_{2g}E_{2g}} = -4.096, \Theta^{1122}_{A_{1g}A_{2g}E_{2g}E_{2g}} = -0.277, \Theta^{1123}_{A_{1g}A_{2g}E_{2g}E_{2g}} = -0.159, \Theta^{1124}_{A_{1g}A_{2g}E_{2g}E_{2g}} = 4.375, \Theta^{1133}_{A_{1g}A_{2g}E_{2g}E_{2g}} = 0.815, \Theta^{1134}_{A_{1g}A_{2g}E_{2g}E_{2g}} = 0.318, \Theta^{1144}_{A_{1g}A_{2g}E_{2g}E_{2g}} = 0.283$

19	$\Theta^{1111}_{A_{1g}E_{2g}E_{2g}E_{2g}} = -0.384, \Theta^{1112}_{A_{1g}E_{2g}E_{2g}E_{2g}} = -0.322, \Theta^{1113}_{A_{1g}E_{2g}E_{2g}E_{2g}} = -1.794, \Theta^{1114}_{A_{1g}E_{2g}E_{2g}E_{2g}} = -0.108, \Theta^{1122}_{A_{1g}E_{2g}E_{2g}E_{2g}} = 0.654, \Theta^{1123}_{A_{1g}E_{2g}E_{2g}E_{2g}} = 0.179, \Theta^{1124}_{A_{1g}E_{2g}E_{2g}E_{2g}} = -4.01, \Theta^{1133}_{A_{1g}E_{2g}E_{2g}E_{2g}} = 1.379, \Theta^{1134}_{A_{1g}E_{2g}E_{2g}E_{2g}} = -0.668, \Theta^{1144}_{A_{1g}E_{2g}E_{2g}E_{2g}} = -0.882, \Theta^{1222}_{A_{1g}E_{2g}E_{2g}E_{2g}} = 0.012, \Theta^{1223}_{A_{1g}E_{2g}E_{2g}E_{2g}} = 2.019, \Theta^{1224}_{A_{1g}E_{2g}E_{2g}E_{2g}} = -0.049, \Theta^{1233}_{A_{1g}E_{2g}E_{2g}E_{2g}} = 0.267, \Theta^{1234}_{A_{1g}E_{2g}E_{2g}E_{2g}} = 1.462, \Theta^{1244}_{A_{1g}E_{2g}E_{2g}E_{2g}} = 0.02, \Theta^{1333}_{A_{1g}E_{2g}E_{2g}E_{2g}} = 0.971, \Theta^{1334}_{A_{1g}E_{2g}E_{2g}E_{2g}} = 0.197, \Theta^{1344}_{A_{1g}E_{2g}E_{2g}E_{2g}} = -3.137, \Theta^{1444}_{A_{1g}E_{2g}E_{2g}E_{2g}} = -0.013$
20	$\Theta^{1111}_{A_{1g}A_{1g}A_{2g}A_{2g}} = 24.0$
21	$\Theta^{1111}_{E_{2g}E_{2g}B_{2u}B_{2u}} = 0.052, \Theta^{1211}_{E_{2g}E_{2g}B_{2u}B_{2u}} = -0.186, \Theta^{1311}_{E_{2g}E_{2g}B_{2u}B_{2u}} = -0.055, \Theta^{1411}_{E_{2g}E_{2g}B_{2u}B_{2u}} = -1.493, \Theta^{2211}_{E_{2g}E_{2g}B_{2u}B_{2u}} = 0.162, \Theta^{2311}_{E_{2g}E_{2g}B_{2u}B_{2u}} = -1.462, \Theta^{2411}_{E_{2g}E_{2g}B_{2u}B_{2u}} = 0.0, \Theta^{3311}_{E_{2g}E_{2g}B_{2u}B_{2u}} = -0.159, \Theta^{3411}_{E_{2g}E_{2g}B_{2u}B_{2u}} = 0.19, \Theta^{4411}_{E_{2g}E_{2g}B_{2u}B_{2u}} = -0.055$
22	$\Theta^{1111}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 7.846, \Theta^{1112}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.387, \Theta^{1113}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -5.335, \Theta^{1122}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 16.06, \Theta^{1123}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 1.866, \Theta^{1124}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 1.528, \Theta^{1133}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 3.275, \Theta^{1134}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.111, \Theta^{1144}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.633, \Theta^{1222}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.419, \Theta^{1223}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -5.718, \Theta^{1224}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.218, \Theta^{1233}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.65, \Theta^{1234}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -2.988, \Theta^{1244}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.028, \Theta^{1333}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.878, \Theta^{1334}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.218, \Theta^{1344}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.391, \Theta^{2222}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 8.227, \Theta^{2223}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 2.221, \Theta^{2224}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 1.882, \Theta^{2233}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 1.388, \Theta^{2234}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.323, \Theta^{2244}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 2.009, \Theta^{2333}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.154, \Theta^{2334}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.622, \Theta^{2344}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.28, \Theta^{2444}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.241, \Theta^{3333}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.091, \Theta^{3334}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.044, \Theta^{3344}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.089, \Theta^{3444}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.017, \Theta^{4444}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.019$

23	$\Theta^{1111}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.033, \Theta^{1112}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.025, \Theta^{1113}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.295, \Theta^{1114}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.026, \Theta^{1122}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.051, \Theta^{1123}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.106, \Theta^{1124}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.005, \Theta^{1133}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.6, \Theta^{1134}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.013, \Theta^{1144}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -1.216, \Theta^{1222}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.034, \Theta^{1223}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.407, \Theta^{1224}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.092, \Theta^{1233}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.224, \Theta^{1234}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.883, \Theta^{1244}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.057, \Theta^{1333}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.7, \Theta^{1334}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.063, \Theta^{1344}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.838, \Theta^{1444}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.0, \Theta^{2222}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.014, \Theta^{2223}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.203, \Theta^{2224}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.112, \Theta^{2233}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -1.191, \Theta^{2234}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.046, \Theta^{2244}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.86, \Theta^{2333}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.316, \Theta^{2334}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.142, \Theta^{2344}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.274, \Theta^{2444}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.255, \Theta^{3333}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.471, \Theta^{3334}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.011, \Theta^{3344}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 1.01, \Theta^{3444}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.018, \Theta^{4444}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.545$
24	$\Theta^{1111}_{E_{2g}E_{2g}B_{2u}E_{1u}} = -0.186, \Theta^{1112}_{E_{2g}E_{2g}B_{2u}E_{1u}} = -0.511, \Theta^{1211}_{E_{2g}E_{2g}B_{2u}E_{1u}} = 1.1, \Theta^{1212}_{E_{2g}E_{2g}B_{2u}E_{1u}} = -0.294, \Theta^{1311}_{E_{2g}E_{2g}B_{2u}E_{1u}} = -0.674, \Theta^{1312}_{E_{2g}E_{2g}B_{2u}E_{1u}} = 0.25, \Theta^{1411}_{E_{2g}E_{2g}B_{2u}E_{1u}} = 0.14, \Theta^{1412}_{E_{2g}E_{2g}B_{2u}E_{1u}} = 0.793, \Theta^{2211}_{E_{2g}E_{2g}B_{2u}E_{1u}} = 0.107, \Theta^{2212}_{E_{2g}E_{2g}B_{2u}E_{1u}} = 0.591, \Theta^{2311}_{E_{2g}E_{2g}B_{2u}E_{1u}} = -0.27, \Theta^{2312}_{E_{2g}E_{2g}B_{2u}E_{1u}} = -0.702, \Theta^{2411}_{E_{2g}E_{2g}B_{2u}E_{1u}} = -0.817, \Theta^{2412}_{E_{2g}E_{2g}B_{2u}E_{1u}} = 0.144, \Theta^{3311}_{E_{2g}E_{2g}B_{2u}E_{1u}} = 0.136, \Theta^{3312}_{E_{2g}E_{2g}B_{2u}E_{1u}} = -0.03, \Theta^{3411}_{E_{2g}E_{2g}B_{2u}E_{1u}} = 0.022, \Theta^{3412}_{E_{2g}E_{2g}B_{2u}E_{1u}} = -0.204, \Theta^{4411}_{E_{2g}E_{2g}B_{2u}E_{1u}} = -0.056, \Theta^{4412}_{E_{2g}E_{2g}B_{2u}E_{1u}} = -0.049$

25	$\Theta^{1111}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.47, \Theta^{1112}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -1.091, \Theta^{1122}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.302, \Theta^{1211}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.035, \Theta^{1212}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -0.029, \Theta^{1222}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 1.487, \Theta^{1311}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -0.617, \Theta^{1312}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -5.285, \Theta^{1322}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.108, \Theta^{1411}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 8.594, \Theta^{1412}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -0.57, \Theta^{1422}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 3.093, \Theta^{2211}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.061, \Theta^{2212}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.349, \Theta^{2222}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -0.088, \Theta^{2311}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 3.127, \Theta^{2312}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.667, \Theta^{2322}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 8.668, \Theta^{2411}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -0.144, \Theta^{2412}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -5.686, \Theta^{2422}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.463, \Theta^{3311}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.135, \Theta^{3312}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 1.045, \Theta^{3322}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -0.055, \Theta^{3411}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -1.408, \Theta^{3412}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.682, \Theta^{3422}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -0.053, \Theta^{4411}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -0.666, \Theta^{4412}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -0.303, \Theta^{4422}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -0.16$
26	$\Theta^{1111}_{A_{1g}E_{2g}B_{2u}E_{1u}} = -0.193, \Theta^{1112}_{A_{1g}E_{2g}B_{2u}E_{1u}} = -2.251, \Theta^{1211}_{A_{1g}E_{2g}B_{2u}E_{1u}} = -0.705, \Theta^{1212}_{A_{1g}E_{2g}B_{2u}E_{1u}} = 0.946, \Theta^{1311}_{A_{1g}E_{2g}B_{2u}E_{1u}} = -0.795, \Theta^{1312}_{A_{1g}E_{2g}B_{2u}E_{1u}} = -11.674, \Theta^{1411}_{A_{1g}E_{2g}B_{2u}E_{1u}} = 11.902, \Theta^{1412}_{A_{1g}E_{2g}B_{2u}E_{1u}} = -0.76$
27	$\Theta^{1111}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.089, \Theta^{1112}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 1.055, \Theta^{1122}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -0.089, \Theta^{1211}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 1.435, \Theta^{1212}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -0.659, \Theta^{1222}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.058, \Theta^{1311}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.411, \Theta^{1312}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 5.28, \Theta^{1322}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -0.303, \Theta^{1411}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 3.137, \Theta^{1412}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.652, \Theta^{1422}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 8.673, \Theta^{2211}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -0.674, \Theta^{2212}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -0.314, \Theta^{2222}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -0.179, \Theta^{2311}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 8.594, \Theta^{2312}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -0.57, \Theta^{2322}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 3.093, \Theta^{2411}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.355, \Theta^{2412}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 5.688, \Theta^{2422}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -0.247, \Theta^{3311}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.49, \Theta^{3312}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -1.088, \Theta^{3322}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.363, \Theta^{3411}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -0.023, \Theta^{3412}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -0.053, \Theta^{3422}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -1.47, \Theta^{4411}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.095, \Theta^{4412}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.347, \Theta^{4422}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -0.095$

28	$\Theta^{1111}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.015, \Theta^{1112}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.012, \Theta^{1113}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.18, \Theta^{1114}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.01, \Theta^{1122}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.015, \Theta^{1123}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.088, \Theta^{1124}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.093, \Theta^{1133}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.833, \Theta^{1134}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.154, \Theta^{1144}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.421, \Theta^{1222}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.007, \Theta^{1223}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.099, \Theta^{1224}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.02, \Theta^{1233}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.195, \Theta^{1234}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.448, \Theta^{1244}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.148, \Theta^{1333}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 1.947, \Theta^{1334}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.365, \Theta^{1344}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 2.02, \Theta^{1444}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.43, \Theta^{2222}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.003, \Theta^{2223}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.035, \Theta^{2224}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.041, \Theta^{2233}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.226, \Theta^{2234}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.029, \Theta^{2244}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.364, \Theta^{2333}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.329, \Theta^{2334}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.636, \Theta^{2344}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.311, \Theta^{2444}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.685, \Theta^{3333}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 2.679, \Theta^{3334}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.099, \Theta^{3344}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 5.52, \Theta^{3444}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.104, \Theta^{4444}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 2.844$
29	$\Theta^{1111}_{E_{2g}E_{2g}B_{2u}E_{1u}} = 0.311, \Theta^{1112}_{E_{2g}E_{2g}B_{2u}E_{1u}} = 0.418, \Theta^{1211}_{E_{2g}E_{2g}B_{2u}E_{1u}} = -0.965, \Theta^{1212}_{E_{2g}E_{2g}B_{2u}E_{1u}} = 0.46, \Theta^{1311}_{E_{2g}E_{2g}B_{2u}E_{1u}} = 1.337, \Theta^{1312}_{E_{2g}E_{2g}B_{2u}E_{1u}} = -0.255, \Theta^{1411}_{E_{2g}E_{2g}B_{2u}E_{1u}} = -0.18, \Theta^{1412}_{E_{2g}E_{2g}B_{2u}E_{1u}} = -1.47, \Theta^{2211}_{E_{2g}E_{2g}B_{2u}E_{1u}} = -0.147, \Theta^{2212}_{E_{2g}E_{2g}B_{2u}E_{1u}} = -0.55, \Theta^{2311}_{E_{2g}E_{2g}B_{2u}E_{1u}} = 0.296, \Theta^{2312}_{E_{2g}E_{2g}B_{2u}E_{1u}} = 1.39, \Theta^{2411}_{E_{2g}E_{2g}B_{2u}E_{1u}} = 1.512, \Theta^{2412}_{E_{2g}E_{2g}B_{2u}E_{1u}} = -0.193, \Theta^{3311}_{E_{2g}E_{2g}B_{2u}E_{1u}} = -0.266, \Theta^{3312}_{E_{2g}E_{2g}B_{2u}E_{1u}} = 0.065, \Theta^{3411}_{E_{2g}E_{2g}B_{2u}E_{1u}} = -0.003, \Theta^{3412}_{E_{2g}E_{2g}B_{2u}E_{1u}} = 0.379, \Theta^{4411}_{E_{2g}E_{2g}B_{2u}E_{1u}} = 0.102, \Theta^{4412}_{E_{2g}E_{2g}B_{2u}E_{1u}} = 0.067$
30	$\Theta^{1111}_{A_{1g}E_{2g}E_{1u}E_{1u}} = 0.706, \Theta^{1112}_{A_{1g}E_{2g}E_{1u}E_{1u}} = 11.39, \Theta^{1122}_{A_{1g}E_{2g}E_{1u}E_{1u}} = -0.706, \Theta^{1211}_{A_{1g}E_{2g}E_{1u}E_{1u}} = -5.749, \Theta^{1212}_{A_{1g}E_{2g}E_{1u}E_{1u}} = 1.624, \Theta^{1222}_{A_{1g}E_{2g}E_{1u}E_{1u}} = 5.749, \Theta^{1311}_{A_{1g}E_{2g}E_{1u}E_{1u}} = -0.7, \Theta^{1312}_{A_{1g}E_{2g}E_{1u}E_{1u}} = -2.042, \Theta^{1322}_{A_{1g}E_{2g}E_{1u}E_{1u}} = 0.7, \Theta^{1411}_{A_{1g}E_{2g}E_{1u}E_{1u}} = -0.353, \Theta^{1412}_{A_{1g}E_{2g}E_{1u}E_{1u}} = 0.382, \Theta^{1422}_{A_{1g}E_{2g}E_{1u}E_{1u}} = 0.353$
31	$\Theta^{1111}_{A_{2g}E_{2g}B_{2u}E_{1u}} = 2.257, \Theta^{1112}_{A_{2g}E_{2g}B_{2u}E_{1u}} = 0.564, \Theta^{1211}_{A_{2g}E_{2g}B_{2u}E_{1u}} = -0.164, \Theta^{1212}_{A_{2g}E_{2g}B_{2u}E_{1u}} = -0.73, \Theta^{1311}_{A_{2g}E_{2g}B_{2u}E_{1u}} = 11.5, \Theta^{1312}_{A_{2g}E_{2g}B_{2u}E_{1u}} = -0.928, \Theta^{1411}_{A_{2g}E_{2g}B_{2u}E_{1u}} = 0.795, \Theta^{1412}_{A_{2g}E_{2g}B_{2u}E_{1u}} = 11.674$

32	$\Theta^{1111}_{A_{2g}A_{2g}E_{2g}E_{2g}} = 11.47, \Theta^{1112}_{A_{2g}A_{2g}E_{2g}E_{2g}} = 0.101, \Theta^{1113}_{A_{2g}A_{2g}E_{2g}E_{2g}} = -4.377, \Theta^{1114}_{A_{2g}A_{2g}E_{2g}E_{2g}} = -1.706, \Theta^{1122}_{A_{2g}A_{2g}E_{2g}E_{2g}} = 11.906, \Theta^{1123}_{A_{2g}A_{2g}E_{2g}E_{2g}} = -0.054, \Theta^{1124}_{A_{2g}A_{2g}E_{2g}E_{2g}} = 1.486, \Theta^{1133}_{A_{2g}A_{2g}E_{2g}E_{2g}} = 0.466, \Theta^{1134}_{A_{2g}A_{2g}E_{2g}E_{2g}} = 0.325, \Theta^{1144}_{A_{2g}A_{2g}E_{2g}E_{2g}} = 0.158$
33	$\Theta^{1111}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.025, \Theta^{1112}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -0.438, \Theta^{1122}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -0.025, \Theta^{1211}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -0.281, \Theta^{1212}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -0.026, \Theta^{1222}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.281, \Theta^{1311}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -0.329, \Theta^{1312}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -2.089, \Theta^{1322}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.329, \Theta^{1411}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 1.088, \Theta^{1412}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -0.598, \Theta^{1422}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -1.088, \Theta^{2211}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.02, \Theta^{2212}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.134, \Theta^{2222}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -0.02, \Theta^{2311}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -1.045, \Theta^{2312}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.38, \Theta^{2322}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 1.045, \Theta^{2411}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -0.177, \Theta^{2412}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -2.144, \Theta^{2422}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.177, \Theta^{3311}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -0.425, \Theta^{3312}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.551, \Theta^{3322}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.425, \Theta^{3411}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -0.4, \Theta^{3412}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -1.616, \Theta^{3422}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.4, \Theta^{4411}_{E_{2g}E_{2g}E_{1u}E_{1u}} = 0.38, \Theta^{4412}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -0.247, \Theta^{4422}_{E_{2g}E_{2g}E_{1u}E_{1u}} = -0.38$
34	$\Theta^{1111}_{E_{2g}E_{2g}B_{1u}E_{1u}} = -0.998, \Theta^{1112}_{E_{2g}E_{2g}B_{1u}E_{1u}} = 0.11, \Theta^{1211}_{E_{2g}E_{2g}B_{1u}E_{1u}} = -0.255, \Theta^{1212}_{E_{2g}E_{2g}B_{1u}E_{1u}} = -2.091, \Theta^{1311}_{E_{2g}E_{2g}B_{1u}E_{1u}} = 0.809, \Theta^{1312}_{E_{2g}E_{2g}B_{1u}E_{1u}} = 0.025, \Theta^{1411}_{E_{2g}E_{2g}B_{1u}E_{1u}} = 0.203, \Theta^{1412}_{E_{2g}E_{2g}B_{1u}E_{1u}} = -0.568, \Theta^{2211}_{E_{2g}E_{2g}B_{1u}E_{1u}} = 1.083, \Theta^{2212}_{E_{2g}E_{2g}B_{1u}E_{1u}} = -0.125, \Theta^{2311}_{E_{2g}E_{2g}B_{1u}E_{1u}} = -0.195, \Theta^{2312}_{E_{2g}E_{2g}B_{1u}E_{1u}} = 0.559, \Theta^{2411}_{E_{2g}E_{2g}B_{1u}E_{1u}} = 0.309, \Theta^{2412}_{E_{2g}E_{2g}B_{1u}E_{1u}} = 0.381, \Theta^{3311}_{E_{2g}E_{2g}B_{1u}E_{1u}} = 1.011, \Theta^{3312}_{E_{2g}E_{2g}B_{1u}E_{1u}} = -0.071, \Theta^{3411}_{E_{2g}E_{2g}B_{1u}E_{1u}} = -0.177, \Theta^{3412}_{E_{2g}E_{2g}B_{1u}E_{1u}} = -2.116, \Theta^{4411}_{E_{2g}E_{2g}B_{1u}E_{1u}} = -1.096, \Theta^{4412}_{E_{2g}E_{2g}B_{1u}E_{1u}} = 0.086$
35	$\Theta^{1111}_{A_{2g}A_{2g}E_{2g}E_{2g}} = 0.773, \Theta^{1112}_{A_{2g}A_{2g}E_{2g}E_{2g}} = 1.522, \Theta^{1113}_{A_{2g}A_{2g}E_{2g}E_{2g}} = -0.509, \Theta^{1114}_{A_{2g}A_{2g}E_{2g}E_{2g}} = 11.686, \Theta^{1122}_{A_{2g}A_{2g}E_{2g}E_{2g}} = -0.027, \Theta^{1123}_{A_{2g}A_{2g}E_{2g}E_{2g}} = 11.795, \Theta^{1124}_{A_{2g}A_{2g}E_{2g}E_{2g}} = 0.319, \Theta^{1133}_{A_{2g}A_{2g}E_{2g}E_{2g}} = 0.08, \Theta^{1134}_{A_{2g}A_{2g}E_{2g}E_{2g}} = -1.462, \Theta^{1144}_{A_{2g}A_{2g}E_{2g}E_{2g}} = -0.825$

36	$\Theta^{1111}_{A_{2g}E_{2g}E_{2g}E_{2g}} = -0.039, \Theta^{1112}_{A_{2g}E_{2g}E_{2g}E_{2g}} = 2.556, \Theta^{1113}_{A_{2g}E_{2g}E_{2g}E_{2g}} = -0.108, \Theta^{1114}_{A_{2g}E_{2g}E_{2g}E_{2g}} = -5.519, \Theta^{1122}_{A_{2g}E_{2g}E_{2g}E_{2g}} = -0.727, \Theta^{1123}_{A_{2g}E_{2g}E_{2g}E_{2g}} = 10.76, \Theta^{1124}_{A_{2g}E_{2g}E_{2g}E_{2g}} = -0.621, \Theta^{1133}_{A_{2g}E_{2g}E_{2g}E_{2g}} = 0.049, \Theta^{1134}_{A_{2g}E_{2g}E_{2g}E_{2g}} = 2.847, \Theta^{1144}_{A_{2g}E_{2g}E_{2g}E_{2g}} = 0.795, \Theta^{1222}_{A_{2g}E_{2g}E_{2g}E_{2g}} = -0.39, \Theta^{1223}_{A_{2g}E_{2g}E_{2g}E_{2g}} = 0.329, \Theta^{1224}_{A_{2g}E_{2g}E_{2g}E_{2g}} = 5.881, \Theta^{1233}_{A_{2g}E_{2g}E_{2g}E_{2g}} = -2.151, \Theta^{1234}_{A_{2g}E_{2g}E_{2g}E_{2g}} = -0.702, \Theta^{1244}_{A_{2g}E_{2g}E_{2g}E_{2g}} = 0.766, \Theta^{1333}_{A_{2g}E_{2g}E_{2g}E_{2g}} = -0.005, \Theta^{1334}_{A_{2g}E_{2g}E_{2g}E_{2g}} = -0.416, \Theta^{1344}_{A_{2g}E_{2g}E_{2g}E_{2g}} = -0.207, \Theta^{1444}_{A_{2g}E_{2g}E_{2g}E_{2g}} = 0.018$
37	$\Theta^{1111}_{B_{1u}E_{1u}E_{1u}E_{1u}} = 5.781, \Theta^{1112}_{B_{1u}E_{1u}E_{1u}E_{1u}} = -3.375, \Theta^{1122}_{B_{1u}E_{1u}E_{1u}E_{1u}} = -17.343, \Theta^{1222}_{B_{1u}E_{1u}E_{1u}E_{1u}} = 1.125$
38	$\Theta^{1111}_{E_{2g}E_{2g}B_{1u}E_{1u}} = 0.09, \Theta^{1112}_{E_{2g}E_{2g}B_{1u}E_{1u}} = 1.072, \Theta^{1211}_{E_{2g}E_{2g}B_{1u}E_{1u}} = -1.47, \Theta^{1212}_{E_{2g}E_{2g}B_{1u}E_{1u}} = -0.251, \Theta^{1311}_{E_{2g}E_{2g}B_{1u}E_{1u}} = 0.203, \Theta^{1312}_{E_{2g}E_{2g}B_{1u}E_{1u}} = 5.369, \Theta^{1411}_{E_{2g}E_{2g}B_{1u}E_{1u}} = 5.6, \Theta^{1412}_{E_{2g}E_{2g}B_{1u}E_{1u}} = -0.329, \Theta^{2211}_{E_{2g}E_{2g}B_{1u}E_{1u}} = 0.356, \Theta^{2212}_{E_{2g}E_{2g}B_{1u}E_{1u}} = -0.396, \Theta^{2311}_{E_{2g}E_{2g}B_{1u}E_{1u}} = -5.527, \Theta^{2312}_{E_{2g}E_{2g}B_{1u}E_{1u}} = 0.439, \Theta^{2411}_{E_{2g}E_{2g}B_{1u}E_{1u}} = 0.459, \Theta^{2412}_{E_{2g}E_{2g}B_{1u}E_{1u}} = 5.705, \Theta^{3311}_{E_{2g}E_{2g}B_{1u}E_{1u}} = -0.542, \Theta^{3312}_{E_{2g}E_{2g}B_{1u}E_{1u}} = -1.041, \Theta^{3411}_{E_{2g}E_{2g}B_{1u}E_{1u}} = -1.416, \Theta^{3412}_{E_{2g}E_{2g}B_{1u}E_{1u}} = 0.649, \Theta^{4411}_{E_{2g}E_{2g}B_{1u}E_{1u}} = 0.096, \Theta^{4412}_{E_{2g}E_{2g}B_{1u}E_{1u}} = 0.365$
39	$\Theta^{1111}_{A_{1g}E_{2g}B_{1u}E_{1u}} = 0.712, \Theta^{1112}_{A_{1g}E_{2g}B_{1u}E_{1u}} = 11.526, \Theta^{1211}_{A_{1g}E_{2g}B_{1u}E_{1u}} = 11.702, \Theta^{1212}_{A_{1g}E_{2g}B_{1u}E_{1u}} = -0.58, \Theta^{1311}_{A_{1g}E_{2g}B_{1u}E_{1u}} = 0.564, \Theta^{1312}_{A_{1g}E_{2g}B_{1u}E_{1u}} = -2.257, \Theta^{1411}_{A_{1g}E_{2g}B_{1u}E_{1u}} = 0.742, \Theta^{1412}_{A_{1g}E_{2g}B_{1u}E_{1u}} = -0.193$
40	$\Theta^{1111}_{A_{1g}A_{1g}E_{2g}E_{2g}} = 0.474, \Theta^{1112}_{A_{1g}A_{1g}E_{2g}E_{2g}} = -0.32, \Theta^{1113}_{A_{1g}A_{1g}E_{2g}E_{2g}} = 4.406, \Theta^{1122}_{A_{1g}A_{1g}E_{2g}E_{2g}} = 0.158, \Theta^{1123}_{A_{1g}A_{1g}E_{2g}E_{2g}} = -1.65, \Theta^{1124}_{A_{1g}A_{1g}E_{2g}E_{2g}} = -1.517, \Theta^{1133}_{A_{1g}A_{1g}E_{2g}E_{2g}} = 11.466, \Theta^{1134}_{A_{1g}A_{1g}E_{2g}E_{2g}} = -0.11, \Theta^{1144}_{A_{1g}A_{1g}E_{2g}E_{2g}} = 11.902$
41	$\Theta^{1111}_{E_{2g}E_{2g}B_{1u}B_{1u}} = 0.71, \Theta^{1211}_{E_{2g}E_{2g}B_{1u}B_{1u}} = 0.055, \Theta^{1311}_{E_{2g}E_{2g}B_{1u}B_{1u}} = -0.565, \Theta^{1411}_{E_{2g}E_{2g}B_{1u}B_{1u}} = 0.108, \Theta^{2211}_{E_{2g}E_{2g}B_{1u}B_{1u}} = 0.743, \Theta^{2311}_{E_{2g}E_{2g}B_{1u}B_{1u}} = 0.319, \Theta^{2411}_{E_{2g}E_{2g}B_{1u}B_{1u}} = 0.196, \Theta^{3311}_{E_{2g}E_{2g}B_{1u}B_{1u}} = -0.694, \Theta^{3411}_{E_{2g}E_{2g}B_{1u}B_{1u}} = 0.0, \Theta^{4411}_{E_{2g}E_{2g}B_{1u}B_{1u}} = -0.758$

42	$\Theta^{1111}_{A_{1g}E_{2g}E_{2g}E_{2g}} = -0.268, \Theta^{1112}_{A_{1g}E_{2g}E_{2g}E_{2g}} = 0.001, \Theta^{1113}_{A_{1g}E_{2g}E_{2g}E_{2g}} = -1.266, \Theta^{1114}_{A_{1g}E_{2g}E_{2g}E_{2g}} = 0.043, \Theta^{1122}_{A_{1g}E_{2g}E_{2g}E_{2g}} = 0.469, \Theta^{1123}_{A_{1g}E_{2g}E_{2g}E_{2g}} = -0.071, \Theta^{1124}_{A_{1g}E_{2g}E_{2g}E_{2g}} = -2.84, \Theta^{1133}_{A_{1g}E_{2g}E_{2g}E_{2g}} = 0.731, \Theta^{1134}_{A_{1g}E_{2g}E_{2g}E_{2g}} = 0.038, \Theta^{1144}_{A_{1g}E_{2g}E_{2g}E_{2g}} = -0.396, \Theta^{1222}_{A_{1g}E_{2g}E_{2g}E_{2g}} = -0.074, \Theta^{1223}_{A_{1g}E_{2g}E_{2g}E_{2g}} = 1.416, \Theta^{1224}_{A_{1g}E_{2g}E_{2g}E_{2g}} = -0.075, \Theta^{1233}_{A_{1g}E_{2g}E_{2g}E_{2g}} = 0.014, \Theta^{1234}_{A_{1g}E_{2g}E_{2g}E_{2g}} = 0.881, \Theta^{1244}_{A_{1g}E_{2g}E_{2g}E_{2g}} = 0.206, \Theta^{1333}_{A_{1g}E_{2g}E_{2g}E_{2g}} = 0.296, \Theta^{1334}_{A_{1g}E_{2g}E_{2g}E_{2g}} = 0.007, \Theta^{1344}_{A_{1g}E_{2g}E_{2g}E_{2g}} = -1.039, \Theta^{1444}_{A_{1g}E_{2g}E_{2g}E_{2g}} = 0.008$
43	$\Theta^{1111}_{A_{1g}A_{1g}E_{2g}E_{2g}} = 11.47, \Theta^{1112}_{A_{1g}A_{1g}E_{2g}E_{2g}} = 0.101, \Theta^{1113}_{A_{1g}A_{1g}E_{2g}E_{2g}} = -4.377, \Theta^{1114}_{A_{1g}A_{1g}E_{2g}E_{2g}} = -1.706, \Theta^{1122}_{A_{1g}A_{1g}E_{2g}E_{2g}} = 11.906, \Theta^{1123}_{A_{1g}A_{1g}E_{2g}E_{2g}} = -0.054, \Theta^{1124}_{A_{1g}A_{1g}E_{2g}E_{2g}} = 1.486, \Theta^{1133}_{A_{1g}A_{1g}E_{2g}E_{2g}} = 0.466, \Theta^{1134}_{A_{1g}A_{1g}E_{2g}E_{2g}} = 0.325, \Theta^{1144}_{A_{1g}A_{1g}E_{2g}E_{2g}} = 0.158$
44	$\Theta^{1111}_{B_{1u}B_{1u}E_{1u}E_{1u}} = 12.0, \Theta^{1122}_{B_{1u}B_{1u}E_{1u}E_{1u}} = 12.0$
45	$\Theta^{1111}_{E_{2g}E_{2g}B_{1u}B_{1u}} = -2.062, \Theta^{1211}_{E_{2g}E_{2g}B_{1u}B_{1u}} = -0.106, \Theta^{1311}_{E_{2g}E_{2g}B_{1u}B_{1u}} = 1.645, \Theta^{1411}_{E_{2g}E_{2g}B_{1u}B_{1u}} = 0.108, \Theta^{2211}_{E_{2g}E_{2g}B_{1u}B_{1u}} = -2.188, \Theta^{2311}_{E_{2g}E_{2g}B_{1u}B_{1u}} = -0.509, \Theta^{2411}_{E_{2g}E_{2g}B_{1u}B_{1u}} = -0.565, \Theta^{3311}_{E_{2g}E_{2g}B_{1u}B_{1u}} = 2.048, \Theta^{3411}_{E_{2g}E_{2g}B_{1u}B_{1u}} = -0.055, \Theta^{4411}_{E_{2g}E_{2g}B_{1u}B_{1u}} = 2.203$
46	$\Theta^{1111}_{E_{2g}E_{2g}B_{1u}B_{2u}} = -2.203, \Theta^{1211}_{E_{2g}E_{2g}B_{1u}B_{2u}} = 0.798, \Theta^{1311}_{E_{2g}E_{2g}B_{1u}B_{2u}} = -10.994, \Theta^{2211}_{E_{2g}E_{2g}B_{1u}B_{2u}} = -0.743, \Theta^{2311}_{E_{2g}E_{2g}B_{1u}B_{2u}} = -0.428, \Theta^{2411}_{E_{2g}E_{2g}B_{1u}B_{2u}} = 11.742, \Theta^{3311}_{E_{2g}E_{2g}B_{1u}B_{2u}} = 2.187, \Theta^{3411}_{E_{2g}E_{2g}B_{1u}B_{2u}} = 0.852, \Theta^{4411}_{E_{2g}E_{2g}B_{1u}B_{2u}} = 0.758$
47	$\Theta^{1111}_{A_{1g}A_{2g}B_{1u}B_{2u}} = 24.0$

48	$\Theta^{1111}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.127, \Theta^{1112}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.054, \Theta^{1113}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.57, \Theta^{1114}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.099, \Theta^{1122}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.319, \Theta^{1123}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.279, \Theta^{1124}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.662, \Theta^{1133}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.965, \Theta^{1134}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.033, \Theta^{1144}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.591, \Theta^{1222}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.023, \Theta^{1223}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.123, \Theta^{1224}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.142, \Theta^{1233}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.19, \Theta^{1234}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 3.429, \Theta^{1244}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.013, \Theta^{1333}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.421, \Theta^{1334}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.186, \Theta^{1344}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.005, \Theta^{1444}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.078, \Theta^{2222}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.171, \Theta^{2223}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.066, \Theta^{2224}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.203, \Theta^{2233}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.626, \Theta^{2234}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.143, \Theta^{2244}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -1.231, \Theta^{2333}_{E_{2g}E_{2g}E_{2g}E_{2g}} = 0.033, \Theta^{2334}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.595, \Theta^{2344}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.254, \Theta^{2444}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.16, \Theta^{3333}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.052, \Theta^{3334}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.035, \Theta^{3344}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.047, \Theta^{3444}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.002, \Theta^{4444}_{E_{2g}E_{2g}E_{2g}E_{2g}} = -0.012$
49	$\Theta^{1111}_{A_{1g}E_{2g}B_{1u}E_{1u}} = -0.172, \Theta^{1112}_{A_{1g}E_{2g}B_{1u}E_{1u}} = -0.58, \Theta^{1211}_{A_{1g}E_{2g}B_{1u}E_{1u}} = -0.544, \Theta^{1212}_{A_{1g}E_{2g}B_{1u}E_{1u}} = 0.072, \Theta^{1311}_{A_{1g}E_{2g}B_{1u}E_{1u}} = -0.73, \Theta^{1312}_{A_{1g}E_{2g}B_{1u}E_{1u}} = 0.164, \Theta^{1411}_{A_{1g}E_{2g}B_{1u}E_{1u}} = -0.084, \Theta^{1412}_{A_{1g}E_{2g}B_{1u}E_{1u}} = -0.705$
50	$\Theta^{1111}_{A_{2g}E_{2g}B_{1u}E_{1u}} = -0.712, \Theta^{1112}_{A_{2g}E_{2g}B_{1u}E_{1u}} = 0.474, \Theta^{1211}_{A_{2g}E_{2g}B_{1u}E_{1u}} = 0.172, \Theta^{1212}_{A_{2g}E_{2g}B_{1u}E_{1u}} = 0.58, \Theta^{1311}_{A_{2g}E_{2g}B_{1u}E_{1u}} = 0.298, \Theta^{1312}_{A_{2g}E_{2g}B_{1u}E_{1u}} = 2.257, \Theta^{1411}_{A_{2g}E_{2g}B_{1u}E_{1u}} = -2.251, \Theta^{1412}_{A_{2g}E_{2g}B_{1u}E_{1u}} = 0.193$
51	$\Theta^{1111}_{A_{2g}E_{2g}B_{1u}E_{1u}} = -2.257, \Theta^{1112}_{A_{2g}E_{2g}B_{1u}E_{1u}} = 0.298, \Theta^{1211}_{A_{2g}E_{2g}B_{1u}E_{1u}} = 0.164, \Theta^{1212}_{A_{2g}E_{2g}B_{1u}E_{1u}} = 2.239, \Theta^{1311}_{A_{2g}E_{2g}B_{1u}E_{1u}} = 0.5, \Theta^{1312}_{A_{2g}E_{2g}B_{1u}E_{1u}} = 0.928, \Theta^{1411}_{A_{2g}E_{2g}B_{1u}E_{1u}} = -0.795, \Theta^{1412}_{A_{2g}E_{2g}B_{1u}E_{1u}} = 0.199$
52	$\Theta^{1111}_{B_{1u}B_{1u}B_{2u}B_{2u}} = 24.0$
53	$\Theta^{1111}_{E_{2g}E_{2g}B_{2u}B_{2u}} = -2.062, \Theta^{1211}_{E_{2g}E_{2g}B_{2u}B_{2u}} = -0.106, \Theta^{1311}_{E_{2g}E_{2g}B_{2u}B_{2u}} = 1.645, \Theta^{1411}_{E_{2g}E_{2g}B_{2u}B_{2u}} = 0.108, \Theta^{2211}_{E_{2g}E_{2g}B_{2u}B_{2u}} = -2.188, \Theta^{2311}_{E_{2g}E_{2g}B_{2u}B_{2u}} = -0.509, \Theta^{2411}_{E_{2g}E_{2g}B_{2u}B_{2u}} = -0.565, \Theta^{3311}_{E_{2g}E_{2g}B_{2u}B_{2u}} = 2.048, \Theta^{3411}_{E_{2g}E_{2g}B_{2u}B_{2u}} = -0.055, \Theta^{4411}_{E_{2g}E_{2g}B_{2u}B_{2u}} = 2.203$
54	$\Theta^{1111}_{A_{2g}A_{2g}E_{2g}E_{2g}} = 0.883, \Theta^{1112}_{A_{2g}A_{2g}E_{2g}E_{2g}} = -0.081, \Theta^{1113}_{A_{2g}A_{2g}E_{2g}E_{2g}} = 4.096, \Theta^{1114}_{A_{2g}A_{2g}E_{2g}E_{2g}} = 1.706, \Theta^{1122}_{A_{2g}A_{2g}E_{2g}E_{2g}} = 0.466, \Theta^{1123}_{A_{2g}A_{2g}E_{2g}E_{2g}} = 0.159, \Theta^{1124}_{A_{2g}A_{2g}E_{2g}E_{2g}} = -1.389, \Theta^{1133}_{A_{2g}A_{2g}E_{2g}E_{2g}} = 11.185, \Theta^{1134}_{A_{2g}A_{2g}E_{2g}E_{2g}} = -0.318, \Theta^{1144}_{A_{2g}A_{2g}E_{2g}E_{2g}} = 11.466$

55	$\Theta^{1111}_{A_{2g}E_{2g}B_{2u}E_{1u}} = 0.712, \Theta^{1112}_{A_{2g}E_{2g}B_{2u}E_{1u}} = 11.526, \Theta^{1211}_{A_{2g}E_{2g}B_{2u}E_{1u}} = 11.702, \Theta^{1212}_{A_{2g}E_{2g}B_{2u}E_{1u}} = -0.58, \Theta^{1311}_{A_{2g}E_{2g}B_{2u}E_{1u}} = 0.564, \Theta^{1312}_{A_{2g}E_{2g}B_{2u}E_{1u}} = -2.257, \Theta^{1411}_{A_{2g}E_{2g}B_{2u}E_{1u}} = 0.742, \Theta^{1412}_{A_{2g}E_{2g}B_{2u}E_{1u}} = -0.193$
56	$\Theta^{1111}_{A_{1g}E_{2g}B_{2u}E_{1u}} = -0.564, \Theta^{1112}_{A_{1g}E_{2g}B_{2u}E_{1u}} = 2.257, \Theta^{1211}_{A_{1g}E_{2g}B_{2u}E_{1u}} = 0.73, \Theta^{1212}_{A_{1g}E_{2g}B_{2u}E_{1u}} = -0.164, \Theta^{1311}_{A_{1g}E_{2g}B_{2u}E_{1u}} = 0.928, \Theta^{1312}_{A_{1g}E_{2g}B_{2u}E_{1u}} = 11.5, \Theta^{1411}_{A_{1g}E_{2g}B_{2u}E_{1u}} = -11.674, \Theta^{1412}_{A_{1g}E_{2g}B_{2u}E_{1u}} = 0.795$
57	$\Theta^{1111}_{E_{1u}E_{1u}E_{1u}E_{1u}} = 3.0, \Theta^{1122}_{E_{1u}E_{1u}E_{1u}E_{1u}} = 6.0, \Theta^{2222}_{E_{1u}E_{1u}E_{1u}E_{1u}} = 3.0$
58	$\Theta^{1111}_{A_{2g}A_{2g}B_{2u}B_{2u}} = 24.0$
59	$\Theta^{1111}_{E_{2g}E_{2g}B_{1u}B_{1u}} = 11.173, \Theta^{1211}_{E_{2g}E_{2g}B_{1u}B_{1u}} = 0.299, \Theta^{1311}_{E_{2g}E_{2g}B_{1u}B_{1u}} = -4.125, \Theta^{2211}_{E_{2g}E_{2g}B_{1u}B_{1u}} = 11.47, \Theta^{2311}_{E_{2g}E_{2g}B_{1u}B_{1u}} = 1.545, \Theta^{2411}_{E_{2g}E_{2g}B_{1u}B_{1u}} = 1.42, \Theta^{3311}_{E_{2g}E_{2g}B_{1u}B_{1u}} = 0.883, \Theta^{3411}_{E_{2g}E_{2g}B_{1u}B_{1u}} = 0.103, \Theta^{4411}_{E_{2g}E_{2g}B_{1u}B_{1u}} = 0.474$
60	$\Theta^{1111}_{B_{1u}B_{1u}B_{1u}B_{1u}} = 24.0$
61	$\Theta^{1111}_{A_{1g}A_{1g}B_{1u}B_{1u}} = 24.0$
62	$\Theta^{1111}_{E_{2g}E_{2g}B_{2u}B_{2u}} = 11.173, \Theta^{1211}_{E_{2g}E_{2g}B_{2u}B_{2u}} = 0.299, \Theta^{1311}_{E_{2g}E_{2g}B_{2u}B_{2u}} = -4.125, \Theta^{2211}_{E_{2g}E_{2g}B_{2u}B_{2u}} = 11.47, \Theta^{2311}_{E_{2g}E_{2g}B_{2u}B_{2u}} = 1.545, \Theta^{2411}_{E_{2g}E_{2g}B_{2u}B_{2u}} = 1.42, \Theta^{3311}_{E_{2g}E_{2g}B_{2u}B_{2u}} = 0.883, \Theta^{3411}_{E_{2g}E_{2g}B_{2u}B_{2u}} = 0.103, \Theta^{4411}_{E_{2g}E_{2g}B_{2u}B_{2u}} = 0.474$
63	$\Theta^{1111}_{A_{1g}A_{1g}A_{1g}A_{1g}} = 24.0$
64	$\Theta^{1111}_{B_{2u}B_{2u}E_{1u}E_{1u}} = 12.0, \Theta^{1122}_{B_{2u}B_{2u}E_{1u}E_{1u}} = 12.0$
65	$\Theta^{1111}_{A_{2g}A_{2g}A_{2g}A_{2g}} = 24.0$
66	$\Theta^{1111}_{A_{1g}A_{1g}B_{2u}B_{2u}} = 24.0$
67	$\Theta^{1111}_{B_{2u}E_{1u}E_{1u}E_{1u}} = 0.219, \Theta^{1112}_{B_{2u}E_{1u}E_{1u}E_{1u}} = 3.375, \Theta^{1122}_{B_{2u}E_{1u}E_{1u}E_{1u}} = -0.657, \Theta^{1222}_{B_{2u}E_{1u}E_{1u}E_{1u}} = -1.125$
68	$\Theta^{1111}_{B_{2u}B_{2u}B_{2u}B_{2u}} = 24.0$
69	$\Theta^{1111}_{A_{2g}A_{2g}B_{1u}B_{1u}} = 24.0$
70	$\Theta^{1111}_{A_{1g}A_{1g}E_{1u}E_{1u}} = 12.0, \Theta^{1122}_{A_{1g}A_{1g}E_{1u}E_{1u}} = 12.0$

Table E.3: Clebsch-Gordan Coefficients for 3rd order terms of PbTe

Term Index	Clebsh-Gordan Coefficients
1	$\Theta^{111}_{A_{1g}A_{1g}A_{1g}} = 8.0, \Theta^{111}_{T_{1g}T_{1g}T_{1g}} = -8.0, \Theta^{222}_{T_{2g}T_{2g}T_{2g}} = 8.0, \Theta^{222}_{T_{1u}T_{1u}T_{1u}} = -8.0, \Theta^{666}_{T_{1u}T_{1u}T_{1u}} = 8.0, \Theta^{333}_{T_{2u}T_{2u}T_{2u}} = -8.0$
2	$\Theta^{111}_{A_{1g}A_{1g}T_{1g}} = 8.0, \Theta^{111}_{A_{1g}T_{1g}T_{1g}} = -8.0, \Theta^{222}_{T_{2g}T_{2g}T_{1u}} = 8.0, \Theta^{222}_{T_{2g}T_{1u}T_{1u}} = -8.0, \Theta^{663}_{T_{1u}T_{1u}T_{2u}} = 8.0, \Theta^{633}_{T_{1u}T_{2u}T_{2u}} = -8.0$
3	$\Theta^{111}_{A_{1g}A_{1g}T_{2g}} = 2.0, \Theta^{111}_{A_{1g}A_{1g}T_{1u}} = 2.0, \Theta^{114}_{A_{1g}A_{1g}T_{1u}} = 2.0, \Theta^{111}_{A_{1g}A_{1g}T_{2u}} = 2.0, \Theta^{122}_{E_gT_{2g}T_{2g}} = 2.0, \Theta^{122}_{E_gT_{1u}T_{1u}} = -2.0, \Theta^{266}_{E_gT_{1u}T_{1u}} = 2.0, \Theta^{233}_{E_gT_{2u}T_{2u}} = -2.0, \Theta^{111}_{T_{1g}T_{1g}T_{2g}} = -2.0, \Theta^{111}_{T_{1g}T_{1g}T_{1u}} = -2.0, \Theta^{114}_{T_{1g}T_{1g}T_{1u}} = -2.0, \Theta^{111}_{T_{1g}T_{1g}T_{2u}} = -2.0, \Theta^{222}_{T_{1g}T_{2g}T_{2g}} = 2.0, \Theta^{222}_{T_{1g}T_{1u}T_{1u}} = -2.0, \Theta^{366}_{T_{1g}T_{1u}T_{1u}} = 2.0, \Theta^{333}_{T_{1g}T_{2u}T_{2u}} = -2.0, \Theta^{225}_{T_{2g}T_{2g}T_{1u}} = 2.0, \Theta^{222}_{T_{2g}T_{2g}T_{2u}} = 2.0, \Theta^{366}_{T_{2g}T_{1u}T_{1u}} = 2.0, \Theta^{333}_{T_{2g}T_{2u}T_{2u}} = -2.0, \Theta^{225}_{T_{1u}T_{1u}T_{1u}} = -2.0, \Theta^{222}_{T_{1u}T_{1u}T_{2u}} = -2.0, \Theta^{366}_{T_{1u}T_{1u}T_{1u}} = 2.0, \Theta^{333}_{T_{1u}T_{2u}T_{2u}} = -2.0$
4	$\Theta^{112}_{A_{1g}A_{1g}T_{2g}} = 2.0, \Theta^{112}_{A_{1g}A_{1g}T_{1u}} = -2.0, \Theta^{116}_{A_{1g}A_{1g}T_{1u}} = 2.0, \Theta^{113}_{A_{1g}A_{1g}T_{2u}} = -2.0, \Theta^{122}_{A_{1g}T_{2g}T_{2g}} = 2.0, \Theta^{122}_{A_{1g}T_{1u}T_{1u}} = 2.0, \Theta^{166}_{A_{1g}T_{1u}T_{1u}} = 2.0, \Theta^{133}_{A_{1g}T_{2u}T_{2u}} = 2.0, \Theta^{112}_{T_{1g}T_{1g}T_{2g}} = 2.0, \Theta^{112}_{T_{1g}T_{1g}T_{1u}} = -2.0, \Theta^{116}_{T_{1g}T_{1g}T_{1u}} = 2.0, \Theta^{113}_{T_{1g}T_{1g}T_{2u}} = -2.0, \Theta^{122}_{T_{1g}T_{2g}T_{2g}} = -2.0, \Theta^{122}_{T_{1g}T_{1u}T_{1u}} = -2.0, \Theta^{166}_{T_{1g}T_{1u}T_{1u}} = -2.0, \Theta^{133}_{T_{1g}T_{2u}T_{2u}} = -2.0, \Theta^{226}_{T_{2g}T_{2g}T_{1u}} = 2.0, \Theta^{223}_{T_{2g}T_{2g}T_{2u}} = -2.0, \Theta^{266}_{T_{2g}T_{1u}T_{1u}} = 2.0, \Theta^{233}_{T_{2g}T_{2u}T_{2u}} = 2.0, \Theta^{226}_{T_{1u}T_{1u}T_{1u}} = 2.0, \Theta^{223}_{T_{1u}T_{1u}T_{2u}} = -2.0, \Theta^{266}_{T_{1u}T_{1u}T_{1u}} = -2.0, \Theta^{233}_{T_{1u}T_{2u}T_{2u}} = -2.0$
5	$\Theta^{111}_{A_{1g}E_gE_g} = 4.0, \Theta^{122}_{A_{1g}E_gE_g} = 4.0, \Theta^{122}_{T_{1g}T_{1g}T_{1g}} = -4.0, \Theta^{133}_{T_{1g}T_{1g}T_{1g}} = -4.0, \Theta^{112}_{T_{2g}T_{2g}T_{2g}} = 4.0, \Theta^{233}_{T_{2g}T_{2g}T_{2g}} = 4.0, \Theta^{112}_{T_{1u}T_{1u}T_{1u}} = -4.0, \Theta^{233}_{T_{1u}T_{1u}T_{1u}} = -4.0, \Theta^{446}_{T_{1u}T_{1u}T_{1u}} = 4.0, \Theta^{556}_{T_{1u}T_{1u}T_{1u}} = 4.0, \Theta^{113}_{T_{2u}T_{2u}T_{2u}} = -4.0, \Theta^{223}_{T_{2u}T_{2u}T_{2u}} = -4.0$
6	$\Theta^{112}_{A_{1g}E_gT_{1g}} = 4.0, \Theta^{123}_{A_{1g}E_gT_{1g}} = 4.0, \Theta^{112}_{E_gT_{1g}T_{1g}} = -4.0, \Theta^{213}_{E_gT_{1g}T_{1g}} = -4.0, \Theta^{121}_{T_{2g}T_{2g}T_{1u}} = 4.0, \Theta^{112}_{T_{2g}T_{1u}T_{1u}} = -4.0, \Theta^{233}_{T_{2g}T_{2g}T_{1u}} = 4.0, \Theta^{323}_{T_{2g}T_{1u}T_{1u}} = -4.0, \Theta^{461}_{T_{1u}T_{1u}T_{2u}} = 4.0, \Theta^{413}_{T_{1u}T_{2u}T_{2u}} = -4.0, \Theta^{562}_{T_{1u}T_{1u}T_{2u}} = 4.0, \Theta^{523}_{T_{1u}T_{2u}T_{2u}} = -4.0$
7	$\Theta^{111}_{A_{1g}E_gT_{2g}} = 2.0, \Theta^{111}_{A_{1g}E_gT_{1u}} = -2.0, \Theta^{124}_{A_{1g}E_gT_{1u}} = 2.0, \Theta^{121}_{A_{1g}E_gT_{2u}} = -2.0, \Theta^{112}_{E_gT_{2g}T_{2g}} = 2.0, \Theta^{112}_{E_gT_{1u}T_{1u}} = 2.0, \Theta^{246}_{E_gT_{1u}T_{1u}} = 2.0, \Theta^{213}_{E_gT_{2u}T_{2u}} = 2.0, \Theta^{121}_{T_{1g}T_{1g}T_{2g}} = 2.0, \Theta^{121}_{T_{1g}T_{1g}T_{1u}} = -2.0, \Theta^{134}_{T_{1g}T_{1g}T_{1u}} = 2.0, \Theta^{131}_{T_{1g}T_{1g}T_{2u}} = -2.0, \Theta^{212}_{T_{1g}T_{2g}T_{2g}} = -2.0, \Theta^{212}_{T_{1g}T_{1u}T_{1u}} = -2.0, \Theta^{346}_{T_{1g}T_{1u}T_{1u}} = -2.0, \Theta^{313}_{T_{1g}T_{2u}T_{2u}} = -2.0, \Theta^{235}_{T_{2g}T_{2g}T_{1u}} = 2.0, \Theta^{232}_{T_{2g}T_{2g}T_{2u}} = -2.0, \Theta^{356}_{T_{2g}T_{1u}T_{1u}} = 2.0, \Theta^{323}_{T_{2g}T_{2u}T_{2u}} = 2.0, \Theta^{235}_{T_{1u}T_{1u}T_{1u}} = 2.0, \Theta^{232}_{T_{1u}T_{1u}T_{2u}} = -2.0, \Theta^{356}_{T_{1u}T_{1u}T_{1u}} = -2.0, \Theta^{323}_{T_{1u}T_{2u}T_{2u}} = -2.0$

8	$\Theta^{112}_{A_{1g}E_gT_{2g}} = 2.0, \Theta^{112}_{A_{1g}E_gT_{1u}} = 2.0, \Theta^{126}_{A_{1g}E_gT_{1u}} = 2.0, \Theta^{123}_{A_{1g}E_gT_{2u}} = 2.0, \Theta^{112}_{A_{1g}T_{2g}T_{2g}} = 2.0, \Theta^{112}_{A_{1g}T_{1u}T_{1u}} = -2.0, \Theta^{146}_{A_{1g}T_{1u}T_{1u}} = 2.0, \Theta^{113}_{A_{1g}T_{2u}T_{2u}} = -2.0, \Theta^{122}_{T_{1g}T_{1g}T_{2g}} = -2.0, \Theta^{122}_{T_{1g}T_{1g}T_{1u}} = -2.0, \Theta^{136}_{T_{1g}T_{1g}T_{1u}} = -2.0, \Theta^{133}_{T_{1g}T_{1g}T_{2u}} = -2.0, \Theta^{112}_{T_{1g}T_{2g}T_{2g}} = 2.0, \Theta^{112}_{T_{1g}T_{1u}T_{1u}} = -2.0, \Theta^{146}_{T_{1g}T_{1u}T_{1u}} = 2.0, \Theta^{113}_{T_{1g}T_{2u}T_{2u}} = -2.0, \Theta^{236}_{T_{2g}T_{2g}T_{1u}} = 2.0, \Theta^{233}_{T_{2g}T_{2g}T_{2u}} = 2.0, \Theta^{256}_{T_{2g}T_{1u}T_{1u}} = 2.0, \Theta^{223}_{T_{2g}T_{2u}T_{2u}} = -2.0, \Theta^{236}_{T_{1u}T_{1u}T_{1u}} = -2.0, \Theta^{233}_{T_{1u}T_{1u}T_{2u}} = -2.0, \Theta^{256}_{T_{1u}T_{1u}T_{1u}} = 2.0, \Theta^{223}_{T_{1u}T_{2u}T_{2u}} = -2.0$
9	$\Theta^{115}_{A_{1g}E_gT_{1u}} = 2.0, \Theta^{112}_{A_{1g}E_gT_{2u}} = 2.0, \Theta^{123}_{A_{1g}E_gT_{2g}} = 2.0, \Theta^{123}_{A_{1g}E_gT_{1u}} = 2.0, \Theta^{156}_{E_gT_{1u}T_{1u}} = 2.0, \Theta^{123}_{E_gT_{2u}T_{2u}} = -2.0, \Theta^{223}_{E_gT_{2g}T_{2g}} = 2.0, \Theta^{223}_{E_gT_{1u}T_{1u}} = -2.0, \Theta^{125}_{T_{1g}T_{1g}T_{1u}} = -2.0, \Theta^{122}_{T_{1g}T_{1g}T_{2u}} = -2.0, \Theta^{133}_{T_{1g}T_{1g}T_{2g}} = -2.0, \Theta^{133}_{T_{1g}T_{1g}T_{1u}} = -2.0, \Theta^{256}_{T_{1g}T_{1u}T_{1u}} = 2.0, \Theta^{223}_{T_{1g}T_{2u}T_{2u}} = -2.0, \Theta^{323}_{T_{1g}T_{2g}T_{2g}} = 2.0, \Theta^{323}_{T_{1g}T_{1u}T_{1u}} = -2.0, \Theta^{124}_{T_{2g}T_{2g}T_{1u}} = 2.0, \Theta^{121}_{T_{2g}T_{2g}T_{2u}} = 2.0, \Theta^{146}_{T_{2g}T_{1u}T_{1u}} = 2.0, \Theta^{113}_{T_{2g}T_{2u}T_{2u}} = -2.0, \Theta^{124}_{T_{1u}T_{1u}T_{1u}} = -2.0, \Theta^{121}_{T_{1u}T_{1u}T_{2u}} = -2.0, \Theta^{146}_{T_{1u}T_{1u}T_{1u}} = 2.0, \Theta^{113}_{T_{1u}T_{2u}T_{2u}} = -2.0$
10	$\Theta^{112}_{A_{1g}T_{1g}T_{2g}} = 4.0, \Theta^{112}_{A_{1g}T_{1g}T_{1u}} = -4.0, \Theta^{116}_{A_{1g}T_{1g}T_{1u}} = 4.0, \Theta^{113}_{A_{1g}T_{1g}T_{2u}} = -4.0, \Theta^{122}_{A_{1g}T_{2g}T_{1u}} = 4.0, \Theta^{163}_{A_{1g}T_{1u}T_{2u}} = 4.0, \Theta^{122}_{T_{1g}T_{2g}T_{1u}} = -4.0, \Theta^{163}_{T_{1g}T_{1u}T_{2u}} = -4.0, \Theta^{226}_{T_{2g}T_{1u}T_{1u}} = 4.0, \Theta^{223}_{T_{2g}T_{1u}T_{2u}} = -4.0, \Theta^{263}_{T_{2g}T_{1u}T_{2u}} = 4.0, \Theta^{263}_{T_{1u}T_{1u}T_{2u}} = -4.0$
11	$\Theta^{122}_{A_{1g}T_{1g}T_{1g}} = 4.0, \Theta^{133}_{A_{1g}T_{1g}T_{1g}} = 4.0, \Theta^{111}_{E_gE_gT_{1g}} = -4.0, \Theta^{221}_{E_gE_gT_{1g}} = -4.0, \Theta^{112}_{T_{2g}T_{2g}T_{1u}} = -4.0, \Theta^{211}_{T_{2g}T_{1u}T_{1u}} = 4.0, \Theta^{233}_{T_{2g}T_{1u}T_{1u}} = 4.0, \Theta^{332}_{T_{2g}T_{2g}T_{1u}} = -4.0, \Theta^{443}_{T_{1u}T_{1u}T_{2u}} = -4.0, \Theta^{553}_{T_{1u}T_{1u}T_{2u}} = -4.0, \Theta^{611}_{T_{1u}T_{2u}T_{2u}} = 4.0, \Theta^{622}_{T_{1u}T_{2u}T_{2u}} = 4.0$
12	$\Theta^{121}_{A_{1g}T_{1g}T_{2g}} = 2.0, \Theta^{121}_{A_{1g}T_{1g}T_{1u}} = -2.0, \Theta^{134}_{A_{1g}T_{1g}T_{1u}} = 2.0, \Theta^{131}_{A_{1g}T_{1g}T_{2u}} = -2.0, \Theta^{111}_{E_gT_{1g}T_{2g}} = 2.0, \Theta^{111}_{E_gT_{1g}T_{1u}} = -2.0, \Theta^{112}_{E_gT_{2g}T_{1u}} = 2.0, \Theta^{121}_{E_gT_{2g}T_{1u}} = 2.0, \Theta^{214}_{E_gT_{1g}T_{1u}} = 2.0, \Theta^{211}_{E_gT_{1g}T_{2u}} = -2.0, \Theta^{243}_{E_gT_{1u}T_{2u}} = 2.0, \Theta^{261}_{E_gT_{1u}T_{2u}} = 2.0, \Theta^{212}_{T_{1g}T_{2g}T_{1u}} = -2.0, \Theta^{221}_{T_{1g}T_{2g}T_{1u}} = -2.0, \Theta^{343}_{T_{1g}T_{1u}T_{2u}} = -2.0, \Theta^{361}_{T_{1g}T_{1u}T_{2u}} = -2.0, \Theta^{235}_{T_{2g}T_{1u}T_{1u}} = 2.0, \Theta^{232}_{T_{2g}T_{1u}T_{2u}} = -2.0, \Theta^{325}_{T_{2g}T_{1u}T_{1u}} = 2.0, \Theta^{322}_{T_{2g}T_{1u}T_{2u}} = -2.0, \Theta^{353}_{T_{2g}T_{1u}T_{2u}} = 2.0, \Theta^{362}_{T_{2g}T_{1u}T_{2u}} = 2.0, \Theta^{353}_{T_{1u}T_{1u}T_{2u}} = -2.0, \Theta^{362}_{T_{1u}T_{1u}T_{2u}} = -2.0$

13	$\Theta^{122}_{A_{1g}T_{1g}T_{2g}} = 2.0, \Theta^{122}_{A_{1g}T_{1g}T_{1u}} = 2.0, \Theta^{136}_{A_{1g}T_{1g}T_{1u}} = 2.0, \Theta^{133}_{A_{1g}T_{1g}T_{2u}} = 2.0, \Theta^{112}_{A_{1g}T_{2g}T_{1u}} = -2.0, \Theta^{121}_{A_{1g}T_{2g}T_{1u}} = 2.0, \Theta^{143}_{A_{1g}T_{1u}T_{2u}} = -2.0, \Theta^{161}_{A_{1g}T_{1u}T_{2u}} = 2.0, \Theta^{112}_{E_gT_{1g}T_{2g}} = -2.0, \Theta^{112}_{E_gT_{1g}T_{1u}} = -2.0, \Theta^{216}_{E_gT_{1g}T_{1u}} = -2.0, \Theta^{213}_{E_gT_{1g}T_{2u}} = -2.0, \Theta^{112}_{T_{1g}T_{2g}T_{1u}} = -2.0, \Theta^{121}_{T_{1g}T_{2g}T_{1u}} = 2.0, \Theta^{143}_{T_{1g}T_{1u}T_{2u}} = -2.0, \Theta^{161}_{T_{1g}T_{1u}T_{2u}} = 2.0, \Theta^{236}_{T_{2g}T_{1u}T_{1u}} = 2.0, \Theta^{233}_{T_{2g}T_{1u}T_{2u}} = 2.0, \Theta^{253}_{T_{2g}T_{1u}T_{2u}} = -2.0, \Theta^{262}_{T_{2g}T_{1u}T_{2u}} = 2.0, \Theta^{326}_{T_{2g}T_{1u}T_{1u}} = -2.0, \Theta^{323}_{T_{2g}T_{1u}T_{2u}} = -2.0, \Theta^{253}_{T_{1u}T_{1u}T_{2u}} = -2.0, \Theta^{262}_{T_{1u}T_{1u}T_{2u}} = 2.0$
14	$\Theta^{125}_{A_{1g}T_{1g}T_{1u}} = 2.0, \Theta^{122}_{A_{1g}T_{1g}T_{2u}} = 2.0, \Theta^{133}_{A_{1g}T_{1g}T_{2g}} = 2.0, \Theta^{133}_{A_{1g}T_{1g}T_{1u}} = 2.0, \Theta^{115}_{E_gT_{1g}T_{1u}} = -2.0, \Theta^{112}_{E_gT_{1g}T_{2u}} = -2.0, \Theta^{153}_{E_gT_{1u}T_{2u}} = -2.0, \Theta^{162}_{E_gT_{1u}T_{2u}} = 2.0, \Theta^{213}_{E_gT_{1g}T_{2g}} = -2.0, \Theta^{213}_{E_gT_{1g}T_{1u}} = -2.0, \Theta^{223}_{E_gT_{2g}T_{1u}} = 2.0, \Theta^{232}_{E_gT_{2g}T_{1u}} = -2.0, \Theta^{253}_{T_{1g}T_{1u}T_{2u}} = -2.0, \Theta^{262}_{T_{1g}T_{1u}T_{2u}} = 2.0, \Theta^{323}_{T_{1g}T_{2g}T_{1u}} = 2.0, \Theta^{332}_{T_{1g}T_{2g}T_{1u}} = -2.0, \Theta^{124}_{T_{2g}T_{1u}T_{1u}} = -2.0, \Theta^{121}_{T_{2g}T_{1u}T_{2u}} = -2.0, \Theta^{143}_{T_{2g}T_{1u}T_{2u}} = -2.0, \Theta^{161}_{T_{2g}T_{1u}T_{2u}} = 2.0, \Theta^{214}_{T_{2g}T_{1u}T_{1u}} = 2.0, \Theta^{211}_{T_{2g}T_{1u}T_{2u}} = 2.0, \Theta^{143}_{T_{1u}T_{1u}T_{2u}} = -2.0, \Theta^{161}_{T_{1u}T_{1u}T_{2u}} = 2.0$
15	$\Theta^{111}_{A_{1g}T_{2g}T_{2g}} = 2.0, \Theta^{111}_{A_{1g}T_{1u}T_{1u}} = 2.0, \Theta^{144}_{A_{1g}T_{1u}T_{1u}} = 2.0, \Theta^{111}_{A_{1g}T_{2u}T_{2u}} = 2.0, \Theta^{112}_{E_gE_gT_{2g}} = 2.0, \Theta^{112}_{E_gE_gT_{1u}} = -2.0, \Theta^{226}_{E_gE_gT_{1u}} = 2.0, \Theta^{223}_{E_gE_gT_{2u}} = -2.0, \Theta^{111}_{T_{1g}T_{2g}T_{2g}} = -2.0, \Theta^{111}_{T_{1g}T_{1u}T_{1u}} = -2.0, \Theta^{144}_{T_{1g}T_{1u}T_{1u}} = -2.0, \Theta^{111}_{T_{1g}T_{2u}T_{2u}} = -2.0, \Theta^{222}_{T_{1g}T_{1g}T_{2g}} = 2.0, \Theta^{222}_{T_{1g}T_{1g}T_{1u}} = -2.0, \Theta^{336}_{T_{1g}T_{1g}T_{1u}} = 2.0, \Theta^{333}_{T_{1g}T_{1g}T_{2u}} = -2.0, \Theta^{255}_{T_{2g}T_{1u}T_{1u}} = 2.0, \Theta^{222}_{T_{2g}T_{2u}T_{2u}} = 2.0, \Theta^{336}_{T_{2g}T_{2g}T_{1u}} = 2.0, \Theta^{333}_{T_{2g}T_{2g}T_{2u}} = -2.0, \Theta^{255}_{T_{1u}T_{1u}T_{1u}} = -2.0, \Theta^{222}_{T_{1u}T_{2u}T_{2u}} = -2.0, \Theta^{336}_{T_{1u}T_{1u}T_{1u}} = 2.0, \Theta^{333}_{T_{1u}T_{1u}T_{2u}} = -2.0$
16	$\Theta^{111}_{A_{1g}T_{2g}T_{1u}} = 4.0, \Theta^{141}_{A_{1g}T_{1u}T_{2u}} = 4.0, \Theta^{122}_{E_gT_{1g}T_{2g}} = 4.0, \Theta^{122}_{E_gT_{1g}T_{1u}} = -4.0, \Theta^{236}_{E_gT_{1g}T_{1u}} = 4.0, \Theta^{233}_{E_gT_{1g}T_{2u}} = -4.0, \Theta^{111}_{T_{1g}T_{2g}T_{1u}} = -4.0, \Theta^{141}_{T_{1g}T_{1u}T_{2u}} = -4.0, \Theta^{252}_{T_{2g}T_{1u}T_{2u}} = 4.0, \Theta^{336}_{T_{2g}T_{1u}T_{1u}} = 4.0, \Theta^{333}_{T_{2g}T_{1u}T_{2u}} = -4.0, \Theta^{252}_{T_{1u}T_{1u}T_{2u}} = -4.0$
17	$\Theta^{114}_{A_{1g}T_{2g}T_{1u}} = 2.0, \Theta^{111}_{A_{1g}T_{2g}T_{2u}} = 2.0, \Theta^{114}_{A_{1g}T_{1u}T_{1u}} = 2.0, \Theta^{111}_{A_{1g}T_{1u}T_{2u}} = 2.0, \Theta^{125}_{E_gT_{2g}T_{1u}} = 2.0, \Theta^{122}_{E_gT_{2g}T_{2u}} = 2.0, \Theta^{125}_{E_gT_{1u}T_{1u}} = -2.0, \Theta^{122}_{E_gT_{1u}T_{2u}} = -2.0, \Theta^{236}_{E_gT_{2g}T_{1u}} = 2.0, \Theta^{233}_{E_gT_{2g}T_{2u}} = -2.0, \Theta^{236}_{E_gT_{1u}T_{1u}} = 2.0, \Theta^{233}_{E_gT_{1u}T_{2u}} = -2.0, \Theta^{114}_{T_{1g}T_{2g}T_{1u}} = -2.0, \Theta^{111}_{T_{1g}T_{2g}T_{2u}} = -2.0, \Theta^{114}_{T_{1g}T_{1u}T_{1u}} = -2.0, \Theta^{111}_{T_{1g}T_{1u}T_{2u}} = -2.0, \Theta^{225}_{T_{1g}T_{2g}T_{1u}} = 2.0, \Theta^{222}_{T_{1g}T_{2g}T_{2u}} = 2.0, \Theta^{225}_{T_{1g}T_{1u}T_{1u}} = -2.0, \Theta^{222}_{T_{1g}T_{1u}T_{2u}} = -2.0, \Theta^{336}_{T_{1g}T_{2g}T_{1u}} = 2.0, \Theta^{333}_{T_{1g}T_{2g}T_{2u}} = -2.0, \Theta^{336}_{T_{1g}T_{1u}T_{1u}} = 2.0, \Theta^{333}_{T_{1g}T_{1u}T_{2u}} = -2.0$

18	$\Theta^{115}_{A_{1g}T_{2g}T_{1u}} = 1.0, \Theta^{112}_{A_{1g}T_{2g}T_{2u}} = 1.0, \Theta^{134}_{A_{1g}T_{2g}T_{1u}} = 1.0, \Theta^{131}_{A_{1g}T_{2g}T_{2u}} = -1.0, \Theta^{115}_{A_{1g}T_{1u}T_{1u}} = -1.0, \Theta^{112}_{A_{1g}T_{1u}T_{2u}} = -1.0, \Theta^{134}_{A_{1g}T_{1u}T_{1u}} = 1.0, \Theta^{131}_{A_{1g}T_{1u}T_{2u}} = -1.0, \Theta^{124}_{E_gT_{2g}T_{1u}} = 1.0, \Theta^{121}_{E_gT_{2g}T_{2u}} = 1.0, \Theta^{136}_{E_gT_{2g}T_{1u}} = 1.0, \Theta^{133}_{E_gT_{2g}T_{2u}} = 1.0, \Theta^{124}_{E_gT_{1u}T_{1u}} = 1.0, \Theta^{121}_{E_gT_{1u}T_{2u}} = 1.0, \Theta^{136}_{E_gT_{1u}T_{1u}} = -1.0, \Theta^{133}_{E_gT_{1u}T_{2u}} = -1.0, \Theta^{216}_{E_gT_{2g}T_{1u}} = 1.0, \Theta^{213}_{E_gT_{2g}T_{2u}} = 1.0, \Theta^{225}_{E_gT_{2g}T_{1u}} = 1.0, \Theta^{222}_{E_gT_{2g}T_{2u}} = -1.0, \Theta^{216}_{E_gT_{1u}T_{1u}} = 1.0, \Theta^{213}_{E_gT_{1u}T_{2u}} = 1.0, \Theta^{225}_{E_gT_{1u}T_{1u}} = 1.0, \Theta^{222}_{E_gT_{1u}T_{2u}} = -1.0, \Theta^{115}_{T_{1g}T_{2g}T_{1u}} = 1.0, \Theta^{112}_{T_{1g}T_{2g}T_{2u}} = 1.0, \Theta^{134}_{T_{1g}T_{2g}T_{1u}} = 1.0, \Theta^{131}_{T_{1g}T_{2g}T_{2u}} = -1.0, \Theta^{115}_{T_{1g}T_{1u}T_{1u}} = -1.0, \Theta^{112}_{T_{1g}T_{1u}T_{2u}} = -1.0, \Theta^{134}_{T_{1g}T_{1u}T_{1u}} = 1.0, \Theta^{131}_{T_{1g}T_{1u}T_{2u}} = -1.0, \Theta^{224}_{T_{1g}T_{2g}T_{1u}} = -1.0, \Theta^{221}_{T_{1g}T_{2g}T_{2u}} = -1.0, \Theta^{236}_{T_{1g}T_{2g}T_{1u}} = 1.0, \Theta^{233}_{T_{1g}T_{2g}T_{2u}} = 1.0, \Theta^{224}_{T_{1g}T_{1u}T_{1u}} = -1.0, \Theta^{221}_{T_{1g}T_{1u}T_{2u}} = -1.0, \Theta^{236}_{T_{1g}T_{1u}T_{1u}} = -1.0, \Theta^{233}_{T_{1g}T_{1u}T_{2u}} = -1.0, \Theta^{316}_{T_{1g}T_{2g}T_{1u}} = -1.0, \Theta^{313}_{T_{1g}T_{2g}T_{2u}} = -1.0, \Theta^{325}_{T_{1g}T_{2g}T_{1u}} = 1.0, \Theta^{322}_{T_{1g}T_{2g}T_{2u}} = -1.0, \Theta^{316}_{T_{1g}T_{1u}T_{1u}} = -1.0, \Theta^{313}_{T_{1g}T_{1u}T_{2u}} = -1.0, \Theta^{325}_{T_{1g}T_{1u}T_{1u}} = 1.0, \Theta^{322}_{T_{1g}T_{1u}T_{2u}} = -1.0$
19	$\Theta^{116}_{A_{1g}T_{2g}T_{1u}} = 1.0, \Theta^{113}_{A_{1g}T_{2g}T_{2u}} = -1.0, \Theta^{124}_{A_{1g}T_{2g}T_{1u}} = 1.0, \Theta^{125}_{A_{1g}T_{2g}T_{1u}} = 1.0, \Theta^{121}_{A_{1g}T_{2g}T_{2u}} = 1.0, \Theta^{122}_{A_{1g}T_{2g}T_{2u}} = 1.0, \Theta^{136}_{A_{1g}T_{2g}T_{1u}} = 1.0, \Theta^{133}_{A_{1g}T_{2g}T_{2u}} = 1.0, \Theta^{116}_{A_{1g}T_{1u}T_{1u}} = 1.0, \Theta^{113}_{A_{1g}T_{1u}T_{2u}} = -1.0, \Theta^{124}_{A_{1g}T_{1u}T_{1u}} = -1.0, \Theta^{125}_{A_{1g}T_{1u}T_{1u}} = 1.0, \Theta^{121}_{A_{1g}T_{1u}T_{2u}} = -1.0, \Theta^{122}_{A_{1g}T_{1u}T_{2u}} = 1.0, \Theta^{136}_{A_{1g}T_{1u}T_{1u}} = 1.0, \Theta^{133}_{A_{1g}T_{1u}T_{2u}} = 1.0, \Theta^{126}_{E_gT_{2g}T_{1u}} = 1.0, \Theta^{123}_{E_gT_{2g}T_{2u}} = -1.0, \Theta^{126}_{E_gT_{1u}T_{1u}} = 1.0, \Theta^{123}_{E_gT_{1u}T_{2u}} = -1.0, \Theta^{226}_{E_gT_{2g}T_{1u}} = 1.0, \Theta^{223}_{E_gT_{2g}T_{2u}} = 1.0, \Theta^{226}_{E_gT_{1u}T_{1u}} = -1.0, \Theta^{223}_{E_gT_{1u}T_{2u}} = -1.0, \Theta^{116}_{T_{1g}T_{2g}T_{1u}} = 1.0, \Theta^{113}_{T_{1g}T_{2g}T_{2u}} = -1.0, \Theta^{124}_{T_{1g}T_{2g}T_{1u}} = 1.0, \Theta^{125}_{T_{1g}T_{2g}T_{1u}} = -1.0, \Theta^{121}_{T_{1g}T_{2g}T_{2u}} = 1.0, \Theta^{122}_{T_{1g}T_{2g}T_{2u}} = -1.0, \Theta^{136}_{T_{1g}T_{2g}T_{1u}} = -1.0, \Theta^{133}_{T_{1g}T_{2g}T_{2u}} = -1.0, \Theta^{116}_{T_{1g}T_{1u}T_{1u}} = 1.0, \Theta^{113}_{T_{1g}T_{1u}T_{2u}} = -1.0, \Theta^{124}_{T_{1g}T_{1u}T_{1u}} = -1.0, \Theta^{125}_{T_{1g}T_{1u}T_{1u}} = -1.0, \Theta^{121}_{T_{1g}T_{1u}T_{2u}} = -1.0, \Theta^{122}_{T_{1g}T_{1u}T_{2u}} = -1.0, \Theta^{136}_{T_{1g}T_{1u}T_{1u}} = -1.0, \Theta^{133}_{T_{1g}T_{1u}T_{2u}} = -1.0, \Theta^{226}_{T_{1g}T_{2g}T_{1u}} = 1.0, \Theta^{223}_{T_{1g}T_{2g}T_{2u}} = -1.0, \Theta^{226}_{T_{1g}T_{1u}T_{1u}} = 1.0, \Theta^{223}_{T_{1g}T_{1u}T_{2u}} = -1.0, \Theta^{326}_{T_{1g}T_{2g}T_{1u}} = 1.0, \Theta^{323}_{T_{1g}T_{2g}T_{2u}} = 1.0, \Theta^{326}_{T_{1g}T_{1u}T_{1u}} = -1.0, \Theta^{323}_{T_{1g}T_{1u}T_{2u}} = -1.0$
20	$\Theta^{126}_{A_{1g}T_{2g}T_{1u}} = 6.0, \Theta^{123}_{A_{1g}T_{2g}T_{2u}} = -6.0, \Theta^{126}_{A_{1g}T_{1u}T_{1u}} = -6.0, \Theta^{123}_{A_{1g}T_{1u}T_{2u}} = 6.0, \Theta^{126}_{T_{1g}T_{2g}T_{1u}} = -6.0, \Theta^{123}_{T_{1g}T_{2g}T_{2u}} = 6.0, \Theta^{126}_{T_{1g}T_{1u}T_{1u}} = 6.0, \Theta^{123}_{T_{1g}T_{1u}T_{2u}} = -6.0$

21	$\Theta^{133}_{A_{1g}T_{2g}T_{2g}} = 2.0, \Theta^{133}_{A_{1g}T_{1u}T_{1u}} = 2.0, \Theta^{155}_{A_{1g}T_{1u}T_{1u}} = 2.0, \Theta^{122}_{A_{1g}T_{2u}T_{2u}} = 2.0, \Theta^{116}_{E_gE_gT_{1u}} = 2.0, \Theta^{113}_{E_gE_gT_{2u}} = -2.0, \Theta^{222}_{E_gE_gT_{2g}} = 2.0, \Theta^{222}_{E_gE_gT_{1u}} = -2.0, \Theta^{133}_{T_{1g}T_{2g}T_{2g}} = -2.0, \Theta^{133}_{T_{1g}T_{1u}T_{1u}} = -2.0, \Theta^{155}_{T_{1g}T_{1u}T_{1u}} = -2.0, \Theta^{122}_{T_{1g}T_{2u}T_{2u}} = -2.0, \Theta^{226}_{T_{1g}T_{1g}T_{1u}} = 2.0, \Theta^{223}_{T_{1g}T_{1g}T_{2u}} = -2.0, \Theta^{332}_{T_{1g}T_{1g}T_{2g}} = 2.0, \Theta^{332}_{T_{1g}T_{1g}T_{1u}} = -2.0, \Theta^{116}_{T_{2g}T_{2g}T_{1u}} = 2.0, \Theta^{113}_{T_{2g}T_{2g}T_{2u}} = -2.0, \Theta^{244}_{T_{2g}T_{1u}T_{1u}} = 2.0, \Theta^{211}_{T_{2g}T_{2u}T_{2u}} = 2.0, \Theta^{116}_{T_{1u}T_{1u}T_{1u}} = 2.0, \Theta^{113}_{T_{1u}T_{1u}T_{2u}} = -2.0, \Theta^{244}_{T_{1u}T_{1u}T_{1u}} = -2.0, \Theta^{211}_{T_{1u}T_{2u}T_{2u}} = -2.0$
22	$\Theta^{133}_{A_{1g}T_{2g}T_{1u}} = 4.0, \Theta^{152}_{A_{1g}T_{1u}T_{2u}} = 4.0, \Theta^{126}_{E_gT_{1g}T_{1u}} = 4.0, \Theta^{123}_{E_gT_{1g}T_{2u}} = -4.0, \Theta^{232}_{E_gT_{1g}T_{2g}} = 4.0, \Theta^{232}_{E_gT_{1g}T_{1u}} = -4.0, \Theta^{133}_{T_{1g}T_{2g}T_{1u}} = -4.0, \Theta^{152}_{T_{1g}T_{1u}T_{2u}} = -4.0, \Theta^{116}_{T_{2g}T_{1u}T_{1u}} = 4.0, \Theta^{113}_{T_{2g}T_{1u}T_{2u}} = -4.0, \Theta^{241}_{T_{2g}T_{1u}T_{2u}} = 4.0, \Theta^{241}_{T_{1u}T_{1u}T_{2u}} = -4.0$
23	$\Theta^{135}_{A_{1g}T_{2g}T_{1u}} = 2.0, \Theta^{132}_{A_{1g}T_{2g}T_{2u}} = -2.0, \Theta^{135}_{A_{1g}T_{1u}T_{1u}} = -2.0, \Theta^{132}_{A_{1g}T_{1u}T_{2u}} = 2.0, \Theta^{116}_{E_gT_{2g}T_{1u}} = 2.0, \Theta^{113}_{E_gT_{2g}T_{2u}} = -2.0, \Theta^{116}_{E_gT_{1u}T_{1u}} = -2.0, \Theta^{113}_{E_gT_{1u}T_{2u}} = 2.0, \Theta^{224}_{E_gT_{2g}T_{1u}} = 2.0, \Theta^{221}_{E_gT_{2g}T_{2u}} = -2.0, \Theta^{224}_{E_gT_{1u}T_{1u}} = -2.0, \Theta^{221}_{E_gT_{1u}T_{2u}} = 2.0, \Theta^{135}_{T_{1g}T_{2g}T_{1u}} = -2.0, \Theta^{132}_{T_{1g}T_{2g}T_{2u}} = 2.0, \Theta^{135}_{T_{1g}T_{1u}T_{1u}} = 2.0, \Theta^{132}_{T_{1g}T_{1u}T_{2u}} = -2.0, \Theta^{216}_{T_{1g}T_{2g}T_{1u}} = -2.0, \Theta^{213}_{T_{1g}T_{2g}T_{2u}} = 2.0, \Theta^{216}_{T_{1g}T_{1u}T_{1u}} = 2.0, \Theta^{213}_{T_{1g}T_{1u}T_{2u}} = -2.0, \Theta^{324}_{T_{1g}T_{2g}T_{1u}} = -2.0, \Theta^{321}_{T_{1g}T_{2g}T_{2u}} = 2.0, \Theta^{324}_{T_{1g}T_{1u}T_{1u}} = 2.0, \Theta^{321}_{T_{1g}T_{1u}T_{2u}} = -2.0$
24	$\Theta^{111}_{E_gE_gT_{2g}} = 2.0, \Theta^{111}_{E_gE_gT_{1u}} = 2.0, \Theta^{111}_{E_gT_{2g}T_{2g}} = 2.0, \Theta^{111}_{E_gT_{1u}T_{1u}} = -2.0, \Theta^{224}_{E_gE_gT_{1u}} = 2.0, \Theta^{221}_{E_gE_gT_{2u}} = 2.0, \Theta^{244}_{E_gT_{1u}T_{1u}} = 2.0, \Theta^{211}_{E_gT_{2u}T_{2u}} = -2.0, \Theta^{221}_{T_{1g}T_{1g}T_{2g}} = -2.0, \Theta^{221}_{T_{1g}T_{1g}T_{1u}} = -2.0, \Theta^{211}_{T_{1g}T_{2g}T_{2g}} = 2.0, \Theta^{211}_{T_{1g}T_{1u}T_{1u}} = -2.0, \Theta^{334}_{T_{1g}T_{1g}T_{1u}} = -2.0, \Theta^{331}_{T_{1g}T_{1g}T_{2u}} = -2.0, \Theta^{344}_{T_{1g}T_{1u}T_{1u}} = 2.0, \Theta^{311}_{T_{1g}T_{2u}T_{2u}} = -2.0, \Theta^{335}_{T_{2g}T_{2g}T_{1u}} = 2.0, \Theta^{332}_{T_{2g}T_{2g}T_{2u}} = 2.0, \Theta^{355}_{T_{2g}T_{1u}T_{1u}} = 2.0, \Theta^{322}_{T_{2g}T_{2u}T_{2u}} = -2.0, \Theta^{335}_{T_{1u}T_{1u}T_{1u}} = -2.0, \Theta^{332}_{T_{1u}T_{1u}T_{2u}} = -2.0, \Theta^{355}_{T_{1u}T_{1u}T_{1u}} = 2.0, \Theta^{322}_{T_{1u}T_{2u}T_{2u}} = -2.0$
25	$\Theta^{114}_{E_gE_gT_{1u}} = 2.0, \Theta^{111}_{E_gE_gT_{2u}} = 2.0, \Theta^{133}_{E_gT_{2g}T_{2g}} = 2.0, \Theta^{133}_{E_gT_{1u}T_{1u}} = -2.0, \Theta^{221}_{E_gE_gT_{2g}} = 2.0, \Theta^{221}_{E_gE_gT_{1u}} = 2.0, \Theta^{255}_{E_gT_{1u}T_{1u}} = 2.0, \Theta^{222}_{E_gT_{2u}T_{2u}} = -2.0, \Theta^{224}_{T_{1g}T_{1g}T_{1u}} = -2.0, \Theta^{221}_{T_{1g}T_{1g}T_{2u}} = -2.0, \Theta^{233}_{T_{1g}T_{2g}T_{2g}} = 2.0, \Theta^{233}_{T_{1g}T_{1u}T_{1u}} = -2.0, \Theta^{331}_{T_{1g}T_{1g}T_{2g}} = -2.0, \Theta^{331}_{T_{1g}T_{1g}T_{1u}} = -2.0, \Theta^{355}_{T_{1g}T_{1u}T_{1u}} = 2.0, \Theta^{322}_{T_{1g}T_{2u}T_{2u}} = -2.0, \Theta^{115}_{T_{2g}T_{2g}T_{1u}} = 2.0, \Theta^{112}_{T_{2g}T_{2g}T_{2u}} = 2.0, \Theta^{344}_{T_{2g}T_{1u}T_{1u}} = 2.0, \Theta^{311}_{T_{2g}T_{2u}T_{2u}} = -2.0, \Theta^{115}_{T_{1u}T_{1u}T_{1u}} = -2.0, \Theta^{112}_{T_{1u}T_{1u}T_{2u}} = -2.0, \Theta^{344}_{T_{1u}T_{1u}T_{1u}} = 2.0, \Theta^{311}_{T_{1u}T_{2u}T_{2u}} = -2.0$

26	$\Theta^{123}_{E_gE_gT_{2g}} = 2.0, \Theta^{123}_{E_gE_gT_{1u}} = -2.0, \Theta^{125}_{E_gE_gT_{1u}} = 2.0, \Theta^{122}_{E_gE_gT_{2u}} = -2.0, \Theta^{145}_{E_gT_{1u}T_{1u}} = 2.0, \Theta^{112}_{E_gT_{2u}T_{2u}} = 2.0, \Theta^{213}_{E_gT_{2g}T_{2g}} = 2.0, \Theta^{213}_{E_gT_{1u}T_{1u}} = 2.0, \Theta^{233}_{T_{1g}T_{1g}T_{2g}} = 2.0, \Theta^{233}_{T_{1g}T_{1g}T_{1u}} = -2.0, \Theta^{235}_{T_{1g}T_{1g}T_{1u}} = 2.0, \Theta^{232}_{T_{1g}T_{1g}T_{2u}} = -2.0, \Theta^{245}_{T_{1g}T_{1u}T_{1u}} = -2.0, \Theta^{212}_{T_{1g}T_{2u}T_{2u}} = -2.0, \Theta^{313}_{T_{1g}T_{2g}T_{2g}} = -2.0, \Theta^{313}_{T_{1g}T_{1u}T_{1u}} = -2.0, \Theta^{134}_{T_{2g}T_{2g}T_{1u}} = 2.0, \Theta^{131}_{T_{2g}T_{2g}T_{2u}} = -2.0, \Theta^{145}_{T_{2g}T_{1u}T_{1u}} = 2.0, \Theta^{112}_{T_{2g}T_{2u}T_{2u}} = 2.0, \Theta^{134}_{T_{1u}T_{1u}T_{1u}} = 2.0, \Theta^{131}_{T_{1u}T_{1u}T_{2u}} = -2.0, \Theta^{145}_{T_{1u}T_{1u}T_{1u}} = -2.0, \Theta^{112}_{T_{1u}T_{2u}T_{2u}} = -2.0$
27	$\Theta^{133}_{E_gT_{1g}T_{2g}} = 2.0, \Theta^{133}_{E_gT_{1g}T_{1u}} = -2.0, \Theta^{135}_{E_gT_{1g}T_{1u}} = 2.0, \Theta^{132}_{E_gT_{1g}T_{2u}} = -2.0, \Theta^{142}_{E_gT_{1u}T_{2u}} = 2.0, \Theta^{151}_{E_gT_{1u}T_{2u}} = 2.0, \Theta^{223}_{E_gT_{1g}T_{2g}} = 2.0, \Theta^{223}_{E_gT_{1g}T_{1u}} = -2.0, \Theta^{225}_{E_gT_{1g}T_{1u}} = 2.0, \Theta^{222}_{E_gT_{1g}T_{2u}} = -2.0, \Theta^{213}_{E_gT_{2g}T_{1u}} = 2.0, \Theta^{231}_{E_gT_{2g}T_{1u}} = 2.0, \Theta^{242}_{T_{1g}T_{1u}T_{2u}} = -2.0, \Theta^{251}_{T_{1g}T_{1u}T_{2u}} = -2.0, \Theta^{313}_{T_{1g}T_{2g}T_{1u}} = -2.0, \Theta^{331}_{T_{1g}T_{2g}T_{1u}} = -2.0, \Theta^{134}_{T_{2g}T_{1u}T_{1u}} = 2.0, \Theta^{131}_{T_{2g}T_{1u}T_{2u}} = -2.0, \Theta^{142}_{T_{2g}T_{1u}T_{2u}} = 2.0, \Theta^{151}_{T_{2g}T_{1u}T_{2u}} = 2.0, \Theta^{314}_{T_{2g}T_{1u}T_{1u}} = 2.0, \Theta^{311}_{T_{2g}T_{1u}T_{2u}} = -2.0, \Theta^{142}_{T_{1u}T_{1u}T_{2u}} = -2.0, \Theta^{151}_{T_{1u}T_{1u}T_{2u}} = -2.0$
28	$\Theta^{114}_{E_gT_{2g}T_{1u}} = 1.0, \Theta^{115}_{E_gT_{2g}T_{1u}} = 1.0, \Theta^{111}_{E_gT_{2g}T_{2u}} = 1.0, \Theta^{112}_{E_gT_{2g}T_{2u}} = 1.0, \Theta^{135}_{E_gT_{2g}T_{1u}} = 1.0, \Theta^{132}_{E_gT_{2g}T_{2u}} = -1.0, \Theta^{114}_{E_gT_{1u}T_{1u}} = -1.0, \Theta^{115}_{E_gT_{1u}T_{1u}} = 1.0, \Theta^{111}_{E_gT_{1u}T_{2u}} = -1.0, \Theta^{112}_{E_gT_{1u}T_{2u}} = 1.0, \Theta^{135}_{E_gT_{1u}T_{1u}} = 1.0, \Theta^{132}_{E_gT_{1u}T_{2u}} = -1.0, \Theta^{214}_{E_gT_{2g}T_{1u}} = 1.0, \Theta^{211}_{E_gT_{2g}T_{2u}} = -1.0, \Theta^{234}_{E_gT_{2g}T_{1u}} = 1.0, \Theta^{235}_{E_gT_{2g}T_{1u}} = 1.0, \Theta^{231}_{E_gT_{2g}T_{2u}} = 1.0, \Theta^{232}_{E_gT_{2g}T_{2u}} = 1.0, \Theta^{214}_{E_gT_{1u}T_{1u}} = 1.0, \Theta^{211}_{E_gT_{1u}T_{2u}} = -1.0, \Theta^{234}_{E_gT_{1u}T_{1u}} = 1.0, \Theta^{235}_{E_gT_{1u}T_{1u}} = -1.0, \Theta^{231}_{E_gT_{1u}T_{2u}} = 1.0, \Theta^{232}_{E_gT_{1u}T_{2u}} = -1.0, \Theta^{214}_{T_{1g}T_{2g}T_{1u}} = 1.0, \Theta^{215}_{T_{1g}T_{2g}T_{1u}} = -1.0, \Theta^{211}_{T_{1g}T_{2g}T_{2u}} = 1.0, \Theta^{212}_{T_{1g}T_{2g}T_{2u}} = -1.0, \Theta^{235}_{T_{1g}T_{2g}T_{1u}} = 1.0, \Theta^{232}_{T_{1g}T_{2g}T_{2u}} = -1.0, \Theta^{214}_{T_{1g}T_{1u}T_{1u}} = -1.0, \Theta^{215}_{T_{1g}T_{1u}T_{1u}} = -1.0, \Theta^{211}_{T_{1g}T_{1u}T_{2u}} = -1.0, \Theta^{212}_{T_{1g}T_{1u}T_{2u}} = -1.0, \Theta^{235}_{T_{1g}T_{1u}T_{1u}} = 1.0, \Theta^{232}_{T_{1g}T_{1u}T_{2u}} = -1.0, \Theta^{314}_{T_{1g}T_{2g}T_{1u}} = 1.0, \Theta^{311}_{T_{1g}T_{2g}T_{2u}} = -1.0, \Theta^{334}_{T_{1g}T_{2g}T_{1u}} = -1.0, \Theta^{335}_{T_{1g}T_{2g}T_{1u}} = 1.0, \Theta^{331}_{T_{1g}T_{2g}T_{2u}} = -1.0, \Theta^{332}_{T_{1g}T_{2g}T_{2u}} = 1.0, \Theta^{314}_{T_{1g}T_{1u}T_{1u}} = 1.0, \Theta^{311}_{T_{1g}T_{1u}T_{2u}} = -1.0, \Theta^{334}_{T_{1g}T_{1u}T_{1u}} = -1.0, \Theta^{335}_{T_{1g}T_{1u}T_{1u}} = -1.0, \Theta^{331}_{T_{1g}T_{1u}T_{2u}} = -1.0, \Theta^{332}_{T_{1g}T_{1u}T_{2u}} = -1.0$
29	$\Theta^{134}_{E_gT_{2g}T_{1u}} = 3.0, \Theta^{131}_{E_gT_{2g}T_{2u}} = -3.0, \Theta^{134}_{E_gT_{1u}T_{1u}} = -3.0, \Theta^{131}_{E_gT_{1u}T_{2u}} = 3.0, \Theta^{215}_{E_gT_{2g}T_{1u}} = 3.0, \Theta^{212}_{E_gT_{2g}T_{2u}} = -3.0, \Theta^{215}_{E_gT_{1u}T_{1u}} = -3.0, \Theta^{212}_{E_gT_{1u}T_{2u}} = 3.0, \Theta^{234}_{T_{1g}T_{2g}T_{1u}} = -3.0, \Theta^{231}_{T_{1g}T_{2g}T_{2u}} = 3.0, \Theta^{234}_{T_{1g}T_{1u}T_{1u}} = 3.0, \Theta^{231}_{T_{1g}T_{1u}T_{2u}} = -3.0, \Theta^{315}_{T_{1g}T_{2g}T_{1u}} = -3.0, \Theta^{312}_{T_{1g}T_{2g}T_{2u}} = 3.0, \Theta^{315}_{T_{1g}T_{1u}T_{1u}} = 3.0, \Theta^{312}_{T_{1g}T_{1u}T_{2u}} = -3.0$

Table E.4: Clebsch-Gordan Coefficients for 4th order terms of PbTe

Term Index	Clebsh-Gordan Coefficients
1	$\Theta^{1112}_{T_{1g}T_{1g}T_{1u}T_{2u}} = -5.842, \Theta^{1131}_{T_{1g}T_{1g}T_{1u}T_{2u}} = -5.842, \Theta^{1142}_{T_{1g}T_{1g}T_{1u}T_{2u}} = -8.0, \Theta^{1161}_{T_{1g}T_{1g}T_{1u}T_{2u}} = -8.0, \Theta^{2212}_{T_{1g}T_{1g}T_{1u}T_{2u}} = 5.842, \Theta^{2223}_{T_{1g}T_{1g}T_{1u}T_{2u}} = -5.842, \Theta^{2242}_{T_{1g}T_{1g}T_{1u}T_{2u}} = 8.0, \Theta^{2253}_{T_{1g}T_{1g}T_{1u}T_{2u}} = -8.0, \Theta^{3323}_{T_{1g}T_{1g}T_{1u}T_{2u}} = 5.842, \Theta^{3331}_{T_{1g}T_{1g}T_{1u}T_{2u}} = 5.842, \Theta^{3353}_{T_{1g}T_{1g}T_{1u}T_{2u}} = 8.0, \Theta^{3361}_{T_{1g}T_{1g}T_{1u}T_{2u}} = 8.0$
2	$\Theta^{1111}_{E_gT_{2g}T_{1u}T_{2u}} = -2.921, \Theta^{1132}_{E_gT_{2g}T_{1u}T_{2u}} = 5.842, \Theta^{1141}_{E_gT_{2g}T_{1u}T_{2u}} = -4.0, \Theta^{1162}_{E_gT_{2g}T_{1u}T_{2u}} = 8.0, \Theta^{1213}_{E_gT_{2g}T_{1u}T_{2u}} = -2.921, \Theta^{1222}_{E_gT_{2g}T_{1u}T_{2u}} = -5.842, \Theta^{1243}_{E_gT_{2g}T_{1u}T_{2u}} = -4.0, \Theta^{1252}_{E_gT_{2g}T_{1u}T_{2u}} = -8.0, \Theta^{1321}_{E_gT_{2g}T_{1u}T_{2u}} = -2.921, \Theta^{1333}_{E_gT_{2g}T_{1u}T_{2u}} = -2.921, \Theta^{1351}_{E_gT_{2g}T_{1u}T_{2u}} = -4.0, \Theta^{1363}_{E_gT_{2g}T_{1u}T_{2u}} = -4.0, \Theta^{2111}_{E_gT_{2g}T_{1u}T_{2u}} = 5.06, \Theta^{2141}_{E_gT_{2g}T_{1u}T_{2u}} = 6.928, \Theta^{2213}_{E_gT_{2g}T_{1u}T_{2u}} = -5.06, \Theta^{2243}_{E_gT_{2g}T_{1u}T_{2u}} = -6.928, \Theta^{2321}_{E_gT_{2g}T_{1u}T_{2u}} = 5.06, \Theta^{2333}_{E_gT_{2g}T_{1u}T_{2u}} = -5.06, \Theta^{2351}_{E_gT_{2g}T_{1u}T_{2u}} = 6.928, \Theta^{2363}_{E_gT_{2g}T_{1u}T_{2u}} = -6.928$
3	$\Theta^{1111}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -8.0, \Theta^{1114}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -11.685, \Theta^{1133}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 8.0, \Theta^{1136}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 11.685, \Theta^{1144}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -4.267, \Theta^{1166}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 4.267, \Theta^{2211}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 8.0, \Theta^{2214}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 11.685, \Theta^{2222}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -8.0, \Theta^{2225}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -11.685, \Theta^{2244}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 4.267, \Theta^{2255}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -4.267, \Theta^{3322}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 8.0, \Theta^{3325}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 11.685, \Theta^{3333}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -8.0, \Theta^{3336}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -11.685, \Theta^{3355}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 4.267, \Theta^{3366}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -4.267$
4	$\Theta^{1111}_{E_gT_{1g}T_{1u}T_{2u}} = -2.921, \Theta^{1132}_{E_gT_{1g}T_{1u}T_{2u}} = 2.921, \Theta^{1141}_{E_gT_{1g}T_{1u}T_{2u}} = -4.0, \Theta^{1162}_{E_gT_{1g}T_{1u}T_{2u}} = 4.0, \Theta^{1213}_{E_gT_{1g}T_{1u}T_{2u}} = 2.921, \Theta^{1222}_{E_gT_{1g}T_{1u}T_{2u}} = 2.921, \Theta^{1243}_{E_gT_{1g}T_{1u}T_{2u}} = 4.0, \Theta^{1252}_{E_gT_{1g}T_{1u}T_{2u}} = 4.0, \Theta^{1321}_{E_gT_{1g}T_{1u}T_{2u}} = -5.842, \Theta^{1333}_{E_gT_{1g}T_{1u}T_{2u}} = 5.842, \Theta^{1351}_{E_gT_{1g}T_{1u}T_{2u}} = -8.0, \Theta^{1363}_{E_gT_{1g}T_{1u}T_{2u}} = 8.0, \Theta^{2111}_{E_gT_{1g}T_{1u}T_{2u}} = -5.06, \Theta^{2132}_{E_gT_{1g}T_{1u}T_{2u}} = 5.06, \Theta^{2141}_{E_gT_{1g}T_{1u}T_{2u}} = -6.928, \Theta^{2162}_{E_gT_{1g}T_{1u}T_{2u}} = 6.928, \Theta^{2213}_{E_gT_{1g}T_{1u}T_{2u}} = -5.06, \Theta^{2222}_{E_gT_{1g}T_{1u}T_{2u}} = -5.06, \Theta^{2243}_{E_gT_{1g}T_{1u}T_{2u}} = -6.928, \Theta^{2252}_{E_gT_{1g}T_{1u}T_{2u}} = -6.928$
5	$\Theta^{1112}_{E_gT_{2g}T_{2u}T_{2u}} = 6.928, \Theta^{1223}_{E_gT_{2g}T_{2u}T_{2u}} = -6.928, \Theta^{1313}_{E_gT_{2g}T_{2u}T_{2u}} = 13.856, \Theta^{2112}_{E_gT_{2g}T_{2u}T_{2u}} = 12.0, \Theta^{2223}_{E_gT_{2g}T_{2u}T_{2u}} = 12.0$
6	$\Theta^{1111}_{A_{1g}E_gT_{1g}T_{2g}} = -6.928, \Theta^{1122}_{A_{1g}E_gT_{1g}T_{2g}} = 6.928, \Theta^{1211}_{A_{1g}E_gT_{1g}T_{2g}} = 4.0, \Theta^{1222}_{A_{1g}E_gT_{1g}T_{2g}} = 4.0, \Theta^{1233}_{A_{1g}E_gT_{1g}T_{2g}} = -8.0$
7	$\Theta^{1113}_{A_{1g}T_{2g}T_{1u}T_{1u}} = -8.533, \Theta^{1116}_{A_{1g}T_{2g}T_{1u}T_{1u}} = -11.685, \Theta^{1134}_{A_{1g}T_{2g}T_{1u}T_{1u}} = -11.685, \Theta^{1146}_{A_{1g}T_{2g}T_{1u}T_{1u}} = -16.0, \Theta^{1212}_{A_{1g}T_{2g}T_{1u}T_{1u}} = -8.533, \Theta^{1215}_{A_{1g}T_{2g}T_{1u}T_{1u}} = -11.685, \Theta^{1224}_{A_{1g}T_{2g}T_{1u}T_{1u}} = -11.685, \Theta^{1245}_{A_{1g}T_{2g}T_{1u}T_{1u}} = -16.0, \Theta^{1323}_{A_{1g}T_{2g}T_{1u}T_{1u}} = 8.533, \Theta^{1326}_{A_{1g}T_{2g}T_{1u}T_{1u}} = 11.685, \Theta^{1335}_{A_{1g}T_{2g}T_{1u}T_{1u}} = 11.685, \Theta^{1356}_{A_{1g}T_{2g}T_{1u}T_{1u}} = 16.0$

8	$\Theta^{1111}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 4.267, \Theta^{1133}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 4.267, \Theta^{1411}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 11.685, \Theta^{1433}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 11.685, \Theta^{2211}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 4.267, \Theta^{2222}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 4.267, \Theta^{2511}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 11.685, \Theta^{2522}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 11.685, \Theta^{3322}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 4.267, \Theta^{3333}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 4.267, \Theta^{3622}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 11.685, \Theta^{3633}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 11.685, \Theta^{4411}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 8.0, \Theta^{4433}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 8.0, \Theta^{5511}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 8.0, \Theta^{5522}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 8.0, \Theta^{6622}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 8.0, \Theta^{6633}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 8.0$
9	$\Theta^{1111}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 5.842, \Theta^{1114}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 12.267, \Theta^{1133}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 5.842, \Theta^{1136}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 12.267, \Theta^{1144}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 5.842, \Theta^{1166}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 5.842, \Theta^{2211}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 5.842, \Theta^{2214}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 12.267, \Theta^{2222}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 5.842, \Theta^{2225}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 12.267, \Theta^{2244}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 5.842, \Theta^{2255}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 5.842, \Theta^{3322}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 5.842, \Theta^{3325}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 12.267, \Theta^{3333}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 5.842, \Theta^{3336}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 12.267, \Theta^{3355}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 5.842, \Theta^{3366}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 5.842$
10	$\Theta^{1112}_{T_{1g}T_{2g}T_{1u}T_{2u}} = 5.842, \Theta^{1131}_{T_{1g}T_{2g}T_{1u}T_{2u}} = -5.842, \Theta^{1142}_{T_{1g}T_{2g}T_{1u}T_{2u}} = 8.0, \Theta^{1161}_{T_{1g}T_{2g}T_{1u}T_{2u}} = -8.0, \Theta^{2212}_{T_{1g}T_{2g}T_{1u}T_{2u}} = 5.842, \Theta^{2223}_{T_{1g}T_{2g}T_{1u}T_{2u}} = 5.842, \Theta^{2242}_{T_{1g}T_{2g}T_{1u}T_{2u}} = 8.0, \Theta^{2253}_{T_{1g}T_{2g}T_{1u}T_{2u}} = 8.0, \Theta^{3323}_{T_{1g}T_{2g}T_{1u}T_{2u}} = 5.842, \Theta^{3331}_{T_{1g}T_{2g}T_{1u}T_{2u}} = -5.842, \Theta^{3353}_{T_{1g}T_{2g}T_{1u}T_{2u}} = 8.0, \Theta^{3361}_{T_{1g}T_{2g}T_{1u}T_{2u}} = -8.0$
11	$\Theta^{1111}_{T_{2u}T_{2u}T_{2u}T_{2u}} = 16.0, \Theta^{2222}_{T_{2u}T_{2u}T_{2u}T_{2u}} = 16.0, \Theta^{3333}_{T_{2u}T_{2u}T_{2u}T_{2u}} = 16.0$
12	$\Theta^{1111}_{A_{1g}T_{1g}T_{1u}T_{2u}} = 5.842, \Theta^{1132}_{A_{1g}T_{1g}T_{1u}T_{2u}} = -5.842, \Theta^{1141}_{A_{1g}T_{1g}T_{1u}T_{2u}} = 8.0, \Theta^{1162}_{A_{1g}T_{1g}T_{1u}T_{2u}} = -8.0, \Theta^{1213}_{A_{1g}T_{1g}T_{1u}T_{2u}} = -5.842, \Theta^{1222}_{A_{1g}T_{1g}T_{1u}T_{2u}} = -5.842, \Theta^{1243}_{A_{1g}T_{1g}T_{1u}T_{2u}} = -8.0, \Theta^{1252}_{A_{1g}T_{1g}T_{1u}T_{2u}} = -8.0, \Theta^{1321}_{A_{1g}T_{1g}T_{1u}T_{2u}} = -5.842, \Theta^{1333}_{A_{1g}T_{1g}T_{1u}T_{2u}} = 5.842, \Theta^{1351}_{A_{1g}T_{1g}T_{1u}T_{2u}} = -8.0, \Theta^{1363}_{A_{1g}T_{1g}T_{1u}T_{2u}} = 8.0$
13	$\Theta^{1123}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 5.842, \Theta^{1131}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 5.842, \Theta^{1153}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 4.267, \Theta^{1161}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 4.267, \Theta^{1222}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -5.842, \Theta^{1243}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 12.267, \Theta^{1252}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -12.267, \Theta^{1332}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 5.842, \Theta^{1341}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 12.267, \Theta^{1362}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 12.267, \Theta^{1453}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 8.958, \Theta^{1461}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 8.958, \Theta^{1552}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -5.842, \Theta^{1662}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 5.842, \Theta^{2231}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -5.842, \Theta^{2242}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -4.267, \Theta^{2261}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -4.267, \Theta^{2333}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -5.842, \Theta^{2351}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -12.267, \Theta^{2363}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -12.267, \Theta^{2443}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 5.842, \Theta^{2452}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -8.958, \Theta^{2561}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -8.958, \Theta^{2663}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -5.842, \Theta^{3342}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 4.267, \Theta^{3353}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -4.267, \Theta^{3441}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 5.842, \Theta^{3462}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 8.958, \Theta^{3551}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -5.842, \Theta^{3563}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -8.958, \Theta^{4453}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 4.267, \Theta^{4461}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 4.267, \Theta^{4552}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -4.267, \Theta^{4662}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 4.267, \Theta^{5561}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -4.267, \Theta^{5663}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -4.267$

14	$\Theta^{1111}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 4.267, \Theta^{1114}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 11.685, \Theta^{1133}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 4.267, \Theta^{1136}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 11.685, \Theta^{1144}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 8.0, \Theta^{1166}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 8.0, \Theta^{2211}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 4.267, \Theta^{2214}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 11.685, \Theta^{2222}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 4.267, \Theta^{2225}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 11.685, \Theta^{2244}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 8.0, \Theta^{2255}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 8.0, \Theta^{3322}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 4.267, \Theta^{3325}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 11.685, \Theta^{3333}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 4.267, \Theta^{3336}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 11.685, \Theta^{3355}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 8.0, \Theta^{3366}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 8.0$
15	$\Theta^{1111}_{A_{1g}E_gT_{2g}T_{2g}} = -8.0, \Theta^{1122}_{A_{1g}E_gT_{2g}T_{2g}} = -8.0, \Theta^{1133}_{A_{1g}E_gT_{2g}T_{2g}} = 16.0, \Theta^{1211}_{A_{1g}E_gT_{2g}T_{2g}} = -13.856, \Theta^{1222}_{A_{1g}E_gT_{2g}T_{2g}} = 13.856$
16	$\Theta^{1111}_{A_{1g}T_{2g}T_{1u}T_{2u}} = 5.842, \Theta^{1132}_{A_{1g}T_{2g}T_{1u}T_{2u}} = 5.842, \Theta^{1141}_{A_{1g}T_{2g}T_{1u}T_{2u}} = 8.0, \Theta^{1162}_{A_{1g}T_{2g}T_{1u}T_{2u}} = 8.0, \Theta^{1213}_{A_{1g}T_{2g}T_{1u}T_{2u}} = 5.842, \Theta^{1222}_{A_{1g}T_{2g}T_{1u}T_{2u}} = -5.842, \Theta^{1243}_{A_{1g}T_{2g}T_{1u}T_{2u}} = 8.0, \Theta^{1252}_{A_{1g}T_{2g}T_{1u}T_{2u}} = -8.0, \Theta^{1321}_{A_{1g}T_{2g}T_{1u}T_{2u}} = 5.842, \Theta^{1333}_{A_{1g}T_{2g}T_{1u}T_{2u}} = 5.842, \Theta^{1351}_{A_{1g}T_{2g}T_{1u}T_{2u}} = 8.0, \Theta^{1363}_{A_{1g}T_{2g}T_{1u}T_{2u}} = 8.0$
17	$\Theta^{1223}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 4.267, \Theta^{1226}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 5.842, \Theta^{1235}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 5.842, \Theta^{1256}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 8.0, \Theta^{1312}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 4.267, \Theta^{1315}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 5.842, \Theta^{1324}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 5.842, \Theta^{1345}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 8.0, \Theta^{2123}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -4.267, \Theta^{2126}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -5.842, \Theta^{2135}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -5.842, \Theta^{2156}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -8.0, \Theta^{2313}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -4.267, \Theta^{2316}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -5.842, \Theta^{2334}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -5.842, \Theta^{2346}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -8.0, \Theta^{3112}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -4.267, \Theta^{3115}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -5.842, \Theta^{3124}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -5.842, \Theta^{3145}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -8.0, \Theta^{3213}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 4.267, \Theta^{3216}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 5.842, \Theta^{3234}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 5.842, \Theta^{3246}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 8.0$
18	$\Theta^{1113}_{A_{1g}T_{2g}T_{1u}T_{1u}} = 16.0, \Theta^{1116}_{A_{1g}T_{2g}T_{1u}T_{1u}} = 11.685, \Theta^{1134}_{A_{1g}T_{2g}T_{1u}T_{1u}} = 11.685, \Theta^{1146}_{A_{1g}T_{2g}T_{1u}T_{1u}} = 8.533, \Theta^{1212}_{A_{1g}T_{2g}T_{1u}T_{1u}} = 16.0, \Theta^{1215}_{A_{1g}T_{2g}T_{1u}T_{1u}} = 11.685, \Theta^{1224}_{A_{1g}T_{2g}T_{1u}T_{1u}} = 11.685, \Theta^{1245}_{A_{1g}T_{2g}T_{1u}T_{1u}} = 8.533, \Theta^{1323}_{A_{1g}T_{2g}T_{1u}T_{1u}} = -16.0, \Theta^{1326}_{A_{1g}T_{2g}T_{1u}T_{1u}} = -11.685, \Theta^{1335}_{A_{1g}T_{2g}T_{1u}T_{1u}} = -11.685, \Theta^{1356}_{A_{1g}T_{2g}T_{1u}T_{1u}} = -8.533$
19	$\Theta^{1112}_{T_{1u}T_{2u}T_{2u}T_{2u}} = -8.0, \Theta^{1233}_{T_{1u}T_{2u}T_{2u}T_{2u}} = 8.0, \Theta^{2113}_{T_{1u}T_{2u}T_{2u}T_{2u}} = 8.0, \Theta^{2223}_{T_{1u}T_{2u}T_{2u}T_{2u}} = -8.0, \Theta^{3122}_{T_{1u}T_{2u}T_{2u}T_{2u}} = -8.0, \Theta^{3133}_{T_{1u}T_{2u}T_{2u}T_{2u}} = 8.0, \Theta^{4112}_{T_{1u}T_{2u}T_{2u}T_{2u}} = -5.842, \Theta^{4233}_{T_{1u}T_{2u}T_{2u}T_{2u}} = 5.842, \Theta^{5113}_{T_{1u}T_{2u}T_{2u}T_{2u}} = 5.842, \Theta^{5223}_{T_{1u}T_{2u}T_{2u}T_{2u}} = -5.842, \Theta^{6122}_{T_{1u}T_{2u}T_{2u}T_{2u}} = -5.842, \Theta^{6133}_{T_{1u}T_{2u}T_{2u}T_{2u}} = 5.842$
20	$\Theta^{1133}_{T_{1g}T_{1g}T_{2u}T_{2u}} = 16.0, \Theta^{2211}_{T_{1g}T_{1g}T_{2u}T_{2u}} = 16.0, \Theta^{3322}_{T_{1g}T_{1g}T_{2u}T_{2u}} = 16.0$

21	$\Theta^{1111}_{E_gT_{2g}T_{1u}T_{2u}} = 6.928, \Theta^{1132}_{E_gT_{2g}T_{1u}T_{2u}} = -6.928, \Theta^{1141}_{E_gT_{2g}T_{1u}T_{2u}} = 5.06, \Theta^{1162}_{E_gT_{2g}T_{1u}T_{2u}} = -5.06, \Theta^{1213}_{E_gT_{2g}T_{1u}T_{2u}} = 6.928, \Theta^{1222}_{E_gT_{2g}T_{1u}T_{2u}} = 6.928, \Theta^{1243}_{E_gT_{2g}T_{1u}T_{2u}} = 5.06, \Theta^{1252}_{E_gT_{2g}T_{1u}T_{2u}} = 5.06, \Theta^{2111}_{E_gT_{2g}T_{1u}T_{2u}} = -4.0, \Theta^{2132}_{E_gT_{2g}T_{1u}T_{2u}} = 4.0, \Theta^{2141}_{E_gT_{2g}T_{1u}T_{2u}} = -2.921, \Theta^{2162}_{E_gT_{2g}T_{1u}T_{2u}} = 2.921, \Theta^{2213}_{E_gT_{2g}T_{1u}T_{2u}} = 4.0, \Theta^{2222}_{E_gT_{2g}T_{1u}T_{2u}} = 4.0, \Theta^{2243}_{E_gT_{2g}T_{1u}T_{2u}} = 2.921, \Theta^{2252}_{E_gT_{2g}T_{1u}T_{2u}} = 2.921, \Theta^{2321}_{E_gT_{2g}T_{1u}T_{2u}} = -8.0, \Theta^{2333}_{E_gT_{2g}T_{1u}T_{2u}} = 8.0, \Theta^{2351}_{E_gT_{2g}T_{1u}T_{2u}} = -5.842, \Theta^{2363}_{E_gT_{2g}T_{1u}T_{2u}} = 5.842$
22	$\Theta^{1122}_{E_gE_gT_{1u}T_{1u}} = 6.4, \Theta^{1125}_{E_gE_gT_{1u}T_{1u}} = 17.527, \Theta^{1133}_{E_gE_gT_{1u}T_{1u}} = 6.4, \Theta^{1136}_{E_gE_gT_{1u}T_{1u}} = 17.527, \Theta^{1155}_{E_gE_gT_{1u}T_{1u}} = 12.0, \Theta^{1166}_{E_gE_gT_{1u}T_{1u}} = 12.0, \Theta^{1222}_{E_gE_gT_{1u}T_{1u}} = -7.39, \Theta^{1225}_{E_gE_gT_{1u}T_{1u}} = -20.239, \Theta^{1233}_{E_gE_gT_{1u}T_{1u}} = 7.39, \Theta^{1236}_{E_gE_gT_{1u}T_{1u}} = 20.239, \Theta^{1255}_{E_gE_gT_{1u}T_{1u}} = -13.856, \Theta^{1266}_{E_gE_gT_{1u}T_{1u}} = 13.856, \Theta^{2211}_{E_gE_gT_{1u}T_{1u}} = 8.533, \Theta^{2214}_{E_gE_gT_{1u}T_{1u}} = 23.369, \Theta^{2222}_{E_gE_gT_{1u}T_{1u}} = 2.133, \Theta^{2225}_{E_gE_gT_{1u}T_{1u}} = 5.842, \Theta^{2233}_{E_gE_gT_{1u}T_{1u}} = 2.133, \Theta^{2236}_{E_gE_gT_{1u}T_{1u}} = 5.842, \Theta^{2244}_{E_gE_gT_{1u}T_{1u}} = 16.0, \Theta^{2255}_{E_gE_gT_{1u}T_{1u}} = 4.0, \Theta^{2266}_{E_gE_gT_{1u}T_{1u}} = 4.0$
23	$\Theta^{1122}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 11.685, \Theta^{1422}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 24.533, \Theta^{2233}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 11.685, \Theta^{2533}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 24.533, \Theta^{3311}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 11.685, \Theta^{3611}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 24.533, \Theta^{4422}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 11.685, \Theta^{5533}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 11.685, \Theta^{6611}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 11.685$
24	$\Theta^{1111}_{E_gT_{1g}T_{1u}T_{2u}} = 5.06, \Theta^{1132}_{E_gT_{1g}T_{1u}T_{2u}} = 5.06, \Theta^{1141}_{E_gT_{1g}T_{1u}T_{2u}} = 6.928, \Theta^{1162}_{E_gT_{1g}T_{1u}T_{2u}} = 6.928, \Theta^{1213}_{E_gT_{1g}T_{1u}T_{2u}} = -5.06, \Theta^{1222}_{E_gT_{1g}T_{1u}T_{2u}} = 5.06, \Theta^{1243}_{E_gT_{1g}T_{1u}T_{2u}} = -6.928, \Theta^{1252}_{E_gT_{1g}T_{1u}T_{2u}} = 6.928, \Theta^{2111}_{E_gT_{1g}T_{1u}T_{2u}} = -2.921, \Theta^{2132}_{E_gT_{1g}T_{1u}T_{2u}} = -2.921, \Theta^{2141}_{E_gT_{1g}T_{1u}T_{2u}} = -4.0, \Theta^{2162}_{E_gT_{1g}T_{1u}T_{2u}} = -4.0, \Theta^{2213}_{E_gT_{1g}T_{1u}T_{2u}} = -2.921, \Theta^{2222}_{E_gT_{1g}T_{1u}T_{2u}} = 2.921, \Theta^{2243}_{E_gT_{1g}T_{1u}T_{2u}} = -4.0, \Theta^{2252}_{E_gT_{1g}T_{1u}T_{2u}} = 4.0, \Theta^{2321}_{E_gT_{1g}T_{1u}T_{2u}} = 5.842, \Theta^{2333}_{E_gT_{1g}T_{1u}T_{2u}} = 5.842, \Theta^{2351}_{E_gT_{1g}T_{1u}T_{2u}} = 8.0, \Theta^{2363}_{E_gT_{1g}T_{1u}T_{2u}} = 8.0$
25	$\Theta^{1111}_{T_{1g}T_{1g}T_{2u}T_{2u}} = 8.0, \Theta^{1122}_{T_{1g}T_{1g}T_{2u}T_{2u}} = 8.0, \Theta^{2222}_{T_{1g}T_{1g}T_{2u}T_{2u}} = 8.0, \Theta^{2233}_{T_{1g}T_{1g}T_{2u}T_{2u}} = 8.0, \Theta^{3311}_{T_{1g}T_{1g}T_{2u}T_{2u}} = 8.0, \Theta^{3333}_{T_{1g}T_{1g}T_{2u}T_{2u}} = 8.0$
26	$\Theta^{1111}_{E_gT_{2g}T_{1u}T_{2u}} = 5.06, \Theta^{1141}_{E_gT_{2g}T_{1u}T_{2u}} = 6.928, \Theta^{1213}_{E_gT_{2g}T_{1u}T_{2u}} = 5.06, \Theta^{1243}_{E_gT_{2g}T_{1u}T_{2u}} = 6.928, \Theta^{1321}_{E_gT_{2g}T_{1u}T_{2u}} = -5.06, \Theta^{1333}_{E_gT_{2g}T_{1u}T_{2u}} = -5.06, \Theta^{1351}_{E_gT_{2g}T_{1u}T_{2u}} = -6.928, \Theta^{1363}_{E_gT_{2g}T_{1u}T_{2u}} = -6.928, \Theta^{2111}_{E_gT_{2g}T_{1u}T_{2u}} = 2.921, \Theta^{2132}_{E_gT_{2g}T_{1u}T_{2u}} = 5.842, \Theta^{2141}_{E_gT_{2g}T_{1u}T_{2u}} = 4.0, \Theta^{2162}_{E_gT_{2g}T_{1u}T_{2u}} = 8.0, \Theta^{2213}_{E_gT_{2g}T_{1u}T_{2u}} = -2.921, \Theta^{2222}_{E_gT_{2g}T_{1u}T_{2u}} = 5.842, \Theta^{2243}_{E_gT_{2g}T_{1u}T_{2u}} = -4.0, \Theta^{2252}_{E_gT_{2g}T_{1u}T_{2u}} = 8.0, \Theta^{2321}_{E_gT_{2g}T_{1u}T_{2u}} = -2.921, \Theta^{2333}_{E_gT_{2g}T_{1u}T_{2u}} = 2.921, \Theta^{2351}_{E_gT_{2g}T_{1u}T_{2u}} = -4.0, \Theta^{2363}_{E_gT_{2g}T_{1u}T_{2u}} = 4.0$

27	$\Theta^{1111}_{A_{1g}E_gT_{1u}T_{1u}} = -4.267, \Theta^{1114}_{A_{1g}E_gT_{1u}T_{1u}} = -11.685, \Theta^{1122}_{A_{1g}E_gT_{1u}T_{1u}} = 2.133, \Theta^{1125}_{A_{1g}E_gT_{1u}T_{1u}} = 5.842, \Theta^{1133}_{A_{1g}E_gT_{1u}T_{1u}} = 2.133, \Theta^{1136}_{A_{1g}E_gT_{1u}T_{1u}} = 5.842, \Theta^{1144}_{A_{1g}E_gT_{1u}T_{1u}} = -8.0, \Theta^{1155}_{A_{1g}E_gT_{1u}T_{1u}} = 4.0, \Theta^{1166}_{A_{1g}E_gT_{1u}T_{1u}} = 4.0, \Theta^{1222}_{A_{1g}E_gT_{1u}T_{1u}} = 3.695, \Theta^{1225}_{A_{1g}E_gT_{1u}T_{1u}} = 10.119, \Theta^{1233}_{A_{1g}E_gT_{1u}T_{1u}} = -3.695, \Theta^{1236}_{A_{1g}E_gT_{1u}T_{1u}} = -10.119, \Theta^{1255}_{A_{1g}E_gT_{1u}T_{1u}} = 6.928, \Theta^{1266}_{A_{1g}E_gT_{1u}T_{1u}} = -6.928$
28	$\Theta^{1221}_{T_{1g}T_{1g}T_{1u}T_{2u}} = 8.0, \Theta^{1233}_{T_{1g}T_{1g}T_{1u}T_{2u}} = 8.0, \Theta^{1251}_{T_{1g}T_{1g}T_{1u}T_{2u}} = 5.842, \Theta^{1263}_{T_{1g}T_{1g}T_{1u}T_{2u}} = 5.842, \Theta^{1313}_{T_{1g}T_{1g}T_{1u}T_{2u}} = 8.0, \Theta^{1322}_{T_{1g}T_{1g}T_{1u}T_{2u}} = -8.0, \Theta^{1343}_{T_{1g}T_{1g}T_{1u}T_{2u}} = 5.842, \Theta^{1352}_{T_{1g}T_{1g}T_{1u}T_{2u}} = -5.842, \Theta^{2311}_{T_{1g}T_{1g}T_{1u}T_{2u}} = 8.0, \Theta^{2332}_{T_{1g}T_{1g}T_{1u}T_{2u}} = 8.0, \Theta^{2341}_{T_{1g}T_{1g}T_{1u}T_{2u}} = 5.842, \Theta^{2362}_{T_{1g}T_{1g}T_{1u}T_{2u}} = 5.842$
29	$\Theta^{1112}_{T_{1g}T_{2g}T_{1u}T_{2u}} = 8.0, \Theta^{1131}_{T_{1g}T_{2g}T_{1u}T_{2u}} = -8.0, \Theta^{1142}_{T_{1g}T_{2g}T_{1u}T_{2u}} = 5.842, \Theta^{1161}_{T_{1g}T_{2g}T_{1u}T_{2u}} = -5.842, \Theta^{2212}_{T_{1g}T_{2g}T_{1u}T_{2u}} = 8.0, \Theta^{2223}_{T_{1g}T_{2g}T_{1u}T_{2u}} = 8.0, \Theta^{2242}_{T_{1g}T_{2g}T_{1u}T_{2u}} = 5.842, \Theta^{2253}_{T_{1g}T_{2g}T_{1u}T_{2u}} = 5.842, \Theta^{3323}_{T_{1g}T_{2g}T_{1u}T_{2u}} = 8.0, \Theta^{3331}_{T_{1g}T_{2g}T_{1u}T_{2u}} = -8.0, \Theta^{3353}_{T_{1g}T_{2g}T_{1u}T_{2u}} = 5.842, \Theta^{3361}_{T_{1g}T_{2g}T_{1u}T_{2u}} = -5.842$
30	$\Theta^{1223}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 11.685, \Theta^{1226}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 12.267, \Theta^{1235}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 12.267, \Theta^{1256}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 11.685, \Theta^{1312}_{T_{1g}T_{1g}T_{1u}T_{1u}} = -11.685, \Theta^{1315}_{T_{1g}T_{1g}T_{1u}T_{1u}} = -12.267, \Theta^{1324}_{T_{1g}T_{1g}T_{1u}T_{1u}} = -12.267, \Theta^{1345}_{T_{1g}T_{1g}T_{1u}T_{1u}} = -11.685, \Theta^{2313}_{T_{1g}T_{1g}T_{1u}T_{1u}} = -11.685, \Theta^{2316}_{T_{1g}T_{1g}T_{1u}T_{1u}} = -12.267, \Theta^{2334}_{T_{1g}T_{1g}T_{1u}T_{1u}} = -12.267, \Theta^{2346}_{T_{1g}T_{1g}T_{1u}T_{1u}} = -11.685$
31	$\Theta^{1112}_{E_gT_{1g}T_{2u}T_{2u}} = 12.0, \Theta^{1223}_{E_gT_{1g}T_{2u}T_{2u}} = 12.0, \Theta^{2112}_{E_gT_{1g}T_{2u}T_{2u}} = -6.928, \Theta^{2223}_{E_gT_{1g}T_{2u}T_{2u}} = 6.928, \Theta^{2313}_{E_gT_{1g}T_{2u}T_{2u}} = -13.856$
32	$\Theta^{1111}_{E_gT_{1g}T_{1u}T_{2u}} = 8.0, \Theta^{1132}_{E_gT_{1g}T_{1u}T_{2u}} = 4.0, \Theta^{1141}_{E_gT_{1g}T_{1u}T_{2u}} = 5.842, \Theta^{1162}_{E_gT_{1g}T_{1u}T_{2u}} = 2.921, \Theta^{1213}_{E_gT_{1g}T_{1u}T_{2u}} = -8.0, \Theta^{1222}_{E_gT_{1g}T_{1u}T_{2u}} = 4.0, \Theta^{1243}_{E_gT_{1g}T_{1u}T_{2u}} = -5.842, \Theta^{1252}_{E_gT_{1g}T_{1u}T_{2u}} = 2.921, \Theta^{1321}_{E_gT_{1g}T_{1u}T_{2u}} = 4.0, \Theta^{1333}_{E_gT_{1g}T_{1u}T_{2u}} = -4.0, \Theta^{1351}_{E_gT_{1g}T_{1u}T_{2u}} = 2.921, \Theta^{1363}_{E_gT_{1g}T_{1u}T_{2u}} = -2.921, \Theta^{2132}_{E_gT_{1g}T_{1u}T_{2u}} = -6.928, \Theta^{2162}_{E_gT_{1g}T_{1u}T_{2u}} = -5.06, \Theta^{2222}_{E_gT_{1g}T_{1u}T_{2u}} = 6.928, \Theta^{2252}_{E_gT_{1g}T_{1u}T_{2u}} = 5.06, \Theta^{2321}_{E_gT_{1g}T_{1u}T_{2u}} = 6.928, \Theta^{2333}_{E_gT_{1g}T_{1u}T_{2u}} = 6.928, \Theta^{2351}_{E_gT_{1g}T_{1u}T_{2u}} = 5.06, \Theta^{2363}_{E_gT_{1g}T_{1u}T_{2u}} = 5.06$
33	$\Theta^{1116}_{A_{1g}T_{1g}T_{1u}T_{1u}} = -3.733, \Theta^{1134}_{A_{1g}T_{1g}T_{1u}T_{1u}} = 3.733, \Theta^{1215}_{A_{1g}T_{1g}T_{1u}T_{1u}} = 3.733, \Theta^{1224}_{A_{1g}T_{1g}T_{1u}T_{1u}} = -3.733, \Theta^{1326}_{A_{1g}T_{1g}T_{1u}T_{1u}} = -3.733, \Theta^{1335}_{A_{1g}T_{1g}T_{1u}T_{1u}} = 3.733$

34	$\Theta^{1122}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 8.533, \Theta^{1125}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 17.917, \Theta^{1133}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 8.533, \Theta^{1136}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 17.917, \Theta^{1155}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 10.276, \Theta^{1166}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 10.276, \Theta^{1224}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 17.917, \Theta^{1245}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 34.133, \Theta^{1334}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 17.917, \Theta^{1346}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 34.133, \Theta^{1455}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 17.917, \Theta^{1466}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 17.917, \Theta^{2233}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 8.533, \Theta^{2236}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 17.917, \Theta^{2244}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 10.276, \Theta^{2266}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 10.276, \Theta^{2335}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 17.917, \Theta^{2356}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 34.133, \Theta^{2445}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 17.917, \Theta^{2566}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 17.917, \Theta^{3344}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 10.276, \Theta^{3355}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 10.276, \Theta^{3446}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 17.917, \Theta^{3556}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 17.917, \Theta^{4455}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 8.533, \Theta^{4466}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 8.533, \Theta^{5566}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 8.533$
35	$\Theta^{1111}_{E_gT_{2g}T_{1u}T_{2u}} = 8.0, \Theta^{1132}_{E_gT_{2g}T_{1u}T_{2u}} = -4.0, \Theta^{1141}_{E_gT_{2g}T_{1u}T_{2u}} = 5.842, \Theta^{1162}_{E_gT_{2g}T_{1u}T_{2u}} = -2.921, \Theta^{1213}_{E_gT_{2g}T_{1u}T_{2u}} = 8.0, \Theta^{1222}_{E_gT_{2g}T_{1u}T_{2u}} = 4.0, \Theta^{1243}_{E_gT_{2g}T_{1u}T_{2u}} = 5.842, \Theta^{1252}_{E_gT_{2g}T_{1u}T_{2u}} = 2.921, \Theta^{1321}_{E_gT_{2g}T_{1u}T_{2u}} = -4.0, \Theta^{1333}_{E_gT_{2g}T_{1u}T_{2u}} = -4.0, \Theta^{1351}_{E_gT_{2g}T_{1u}T_{2u}} = -2.921, \Theta^{1363}_{E_gT_{2g}T_{1u}T_{2u}} = -2.921, \Theta^{2132}_{E_gT_{2g}T_{1u}T_{2u}} = 6.928, \Theta^{2162}_{E_gT_{2g}T_{1u}T_{2u}} = 5.06, \Theta^{2222}_{E_gT_{2g}T_{1u}T_{2u}} = 6.928, \Theta^{2252}_{E_gT_{2g}T_{1u}T_{2u}} = 5.06, \Theta^{2321}_{E_gT_{2g}T_{1u}T_{2u}} = -6.928, \Theta^{2333}_{E_gT_{2g}T_{1u}T_{2u}} = 6.928, \Theta^{2351}_{E_gT_{2g}T_{1u}T_{2u}} = -5.06, \Theta^{2363}_{E_gT_{2g}T_{1u}T_{2u}} = 5.06$
36	$\Theta^{1213}_{T_{2g}T_{2g}T_{2u}T_{2u}} = 16.0, \Theta^{1323}_{T_{2g}T_{2g}T_{2u}T_{2u}} = 16.0, \Theta^{2312}_{T_{2g}T_{2g}T_{2u}T_{2u}} = -16.0$
37	$\Theta^{1111}_{E_gE_gT_{1u}T_{1u}} = 5.06, \Theta^{1114}_{E_gE_gT_{1u}T_{1u}} = 10.623, \Theta^{1122}_{E_gE_gT_{1u}T_{1u}} = -2.53, \Theta^{1125}_{E_gE_gT_{1u}T_{1u}} = -5.312, \Theta^{1133}_{E_gE_gT_{1u}T_{1u}} = -2.53, \Theta^{1136}_{E_gE_gT_{1u}T_{1u}} = -5.312, \Theta^{1144}_{E_gE_gT_{1u}T_{1u}} = 5.06, \Theta^{1155}_{E_gE_gT_{1u}T_{1u}} = -2.53, \Theta^{1166}_{E_gE_gT_{1u}T_{1u}} = -2.53, \Theta^{1222}_{E_gE_gT_{1u}T_{1u}} = 8.764, \Theta^{1225}_{E_gE_gT_{1u}T_{1u}} = 18.4, \Theta^{1233}_{E_gE_gT_{1u}T_{1u}} = -8.764, \Theta^{1236}_{E_gE_gT_{1u}T_{1u}} = -18.4, \Theta^{1255}_{E_gE_gT_{1u}T_{1u}} = 8.764, \Theta^{1266}_{E_gE_gT_{1u}T_{1u}} = -8.764, \Theta^{2211}_{E_gE_gT_{1u}T_{1u}} = -5.06, \Theta^{2214}_{E_gE_gT_{1u}T_{1u}} = -10.623, \Theta^{2222}_{E_gE_gT_{1u}T_{1u}} = 2.53, \Theta^{2225}_{E_gE_gT_{1u}T_{1u}} = 5.312, \Theta^{2233}_{E_gE_gT_{1u}T_{1u}} = 2.53, \Theta^{2236}_{E_gE_gT_{1u}T_{1u}} = 5.312, \Theta^{2244}_{E_gE_gT_{1u}T_{1u}} = -5.06, \Theta^{2255}_{E_gE_gT_{1u}T_{1u}} = 2.53, \Theta^{2266}_{E_gE_gT_{1u}T_{1u}} = 2.53$
38	$\Theta^{1111}_{A_{1g}E_gT_{2u}T_{2u}} = -8.0, \Theta^{1122}_{A_{1g}E_gT_{2u}T_{2u}} = 16.0, \Theta^{1133}_{A_{1g}E_gT_{2u}T_{2u}} = -8.0, \Theta^{1211}_{A_{1g}E_gT_{2u}T_{2u}} = 13.856, \Theta^{1233}_{A_{1g}E_gT_{2u}T_{2u}} = -13.856$
39	$\Theta^{1223}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -5.842, \Theta^{1226}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -4.267, \Theta^{1235}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -8.0, \Theta^{1256}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -5.842, \Theta^{1312}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -5.842, \Theta^{1315}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -8.0, \Theta^{1324}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -4.267, \Theta^{1345}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -5.842, \Theta^{2123}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 5.842, \Theta^{2126}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 8.0, \Theta^{2135}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 4.267, \Theta^{2156}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 5.842, \Theta^{2313}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 5.842, \Theta^{2316}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 8.0, \Theta^{2334}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 4.267, \Theta^{2346}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 5.842, \Theta^{3112}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 5.842, \Theta^{3115}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 4.267, \Theta^{3124}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 8.0, \Theta^{3145}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 5.842, \Theta^{3213}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -5.842, \Theta^{3216}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -4.267, \Theta^{3234}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -8.0, \Theta^{3246}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -5.842$

40	$\Theta^{1111}_{E_gE_gT_{1u}T_{1u}} = -3.695, \Theta^{1114}_{E_gE_gT_{1u}T_{1u}} = -10.119, \Theta^{1122}_{E_gE_gT_{1u}T_{1u}} = 1.848, \Theta^{1125}_{E_gE_gT_{1u}T_{1u}} = 5.06, \Theta^{1133}_{E_gE_gT_{1u}T_{1u}} = 1.848, \Theta^{1136}_{E_gE_gT_{1u}T_{1u}} = 5.06, \Theta^{1144}_{E_gE_gT_{1u}T_{1u}} = -6.928, \Theta^{1155}_{E_gE_gT_{1u}T_{1u}} = 3.464, \Theta^{1166}_{E_gE_gT_{1u}T_{1u}} = 3.464, \Theta^{1222}_{E_gE_gT_{1u}T_{1u}} = -6.4, \Theta^{1225}_{E_gE_gT_{1u}T_{1u}} = -17.527, \Theta^{1233}_{E_gE_gT_{1u}T_{1u}} = 6.4, \Theta^{1236}_{E_gE_gT_{1u}T_{1u}} = 17.527, \Theta^{1255}_{E_gE_gT_{1u}T_{1u}} = -12.0, \Theta^{1266}_{E_gE_gT_{1u}T_{1u}} = 12.0, \Theta^{2211}_{E_gE_gT_{1u}T_{1u}} = 3.695, \Theta^{2214}_{E_gE_gT_{1u}T_{1u}} = 10.119, \Theta^{2222}_{E_gE_gT_{1u}T_{1u}} = -1.848, \Theta^{2225}_{E_gE_gT_{1u}T_{1u}} = -5.06, \Theta^{2233}_{E_gE_gT_{1u}T_{1u}} = -1.848, \Theta^{2236}_{E_gE_gT_{1u}T_{1u}} = -5.06, \Theta^{2244}_{E_gE_gT_{1u}T_{1u}} = 6.928, \Theta^{2255}_{E_gE_gT_{1u}T_{1u}} = -3.464, \Theta^{2266}_{E_gE_gT_{1u}T_{1u}} = -3.464$
41	$\Theta^{1112}_{T_{2g}T_{2g}T_{1u}T_{2u}} = -5.842, \Theta^{1131}_{T_{2g}T_{2g}T_{1u}T_{2u}} = -5.842, \Theta^{1142}_{T_{2g}T_{2g}T_{1u}T_{2u}} = -8.0, \Theta^{1161}_{T_{2g}T_{2g}T_{1u}T_{2u}} = -8.0, \Theta^{2212}_{T_{2g}T_{2g}T_{1u}T_{2u}} = 5.842, \Theta^{2223}_{T_{2g}T_{2g}T_{1u}T_{2u}} = -5.842, \Theta^{2242}_{T_{2g}T_{2g}T_{1u}T_{2u}} = 8.0, \Theta^{2253}_{T_{2g}T_{2g}T_{1u}T_{2u}} = -8.0, \Theta^{3323}_{T_{2g}T_{2g}T_{1u}T_{2u}} = 5.842, \Theta^{3331}_{T_{2g}T_{2g}T_{1u}T_{2u}} = 5.842, \Theta^{3353}_{T_{2g}T_{2g}T_{1u}T_{2u}} = 8.0, \Theta^{3361}_{T_{2g}T_{2g}T_{1u}T_{2u}} = 8.0$
42	$\Theta^{1223}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -5.842, \Theta^{1226}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -8.0, \Theta^{1235}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -4.267, \Theta^{1256}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -5.842, \Theta^{1312}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -5.842, \Theta^{1315}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -4.267, \Theta^{1324}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -8.0, \Theta^{1345}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -5.842, \Theta^{2123}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 5.842, \Theta^{2126}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 4.267, \Theta^{2135}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 8.0, \Theta^{2156}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 5.842, \Theta^{2313}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 5.842, \Theta^{2316}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 4.267, \Theta^{2334}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 8.0, \Theta^{2346}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 5.842, \Theta^{3112}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 5.842, \Theta^{3115}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 8.0, \Theta^{3124}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 4.267, \Theta^{3145}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 5.842, \Theta^{3213}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -5.842, \Theta^{3216}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -8.0, \Theta^{3234}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -4.267, \Theta^{3246}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -5.842$
43	$\Theta^{1113}_{E_gT_{2g}T_{1u}T_{1u}} = 5.842, \Theta^{1116}_{E_gT_{2g}T_{1u}T_{1u}} = 6.133, \Theta^{1134}_{E_gT_{2g}T_{1u}T_{1u}} = 6.133, \Theta^{1146}_{E_gT_{2g}T_{1u}T_{1u}} = 5.842, \Theta^{1212}_{E_gT_{2g}T_{1u}T_{1u}} = 5.842, \Theta^{1215}_{E_gT_{2g}T_{1u}T_{1u}} = 6.133, \Theta^{1224}_{E_gT_{2g}T_{1u}T_{1u}} = 6.133, \Theta^{1245}_{E_gT_{2g}T_{1u}T_{1u}} = 5.842, \Theta^{1323}_{E_gT_{2g}T_{1u}T_{1u}} = 11.685, \Theta^{1326}_{E_gT_{2g}T_{1u}T_{1u}} = 12.267, \Theta^{1335}_{E_gT_{2g}T_{1u}T_{1u}} = 12.267, \Theta^{1356}_{E_gT_{2g}T_{1u}T_{1u}} = 11.685, \Theta^{2113}_{E_gT_{2g}T_{1u}T_{1u}} = 10.119, \Theta^{2116}_{E_gT_{2g}T_{1u}T_{1u}} = 10.623, \Theta^{2134}_{E_gT_{2g}T_{1u}T_{1u}} = 10.623, \Theta^{2146}_{E_gT_{2g}T_{1u}T_{1u}} = 10.119, \Theta^{2212}_{E_gT_{2g}T_{1u}T_{1u}} = -10.119, \Theta^{2215}_{E_gT_{2g}T_{1u}T_{1u}} = -10.623, \Theta^{2224}_{E_gT_{2g}T_{1u}T_{1u}} = -10.623, \Theta^{2245}_{E_gT_{2g}T_{1u}T_{1u}} = -10.119$
44	$\Theta^{1111}_{E_gE_gT_{1g}T_{1g}} = 4.0, \Theta^{1122}_{E_gE_gT_{1g}T_{1g}} = 4.0, \Theta^{1133}_{E_gE_gT_{1g}T_{1g}} = 16.0, \Theta^{1211}_{E_gE_gT_{1g}T_{1g}} = 13.856, \Theta^{1222}_{E_gE_gT_{1g}T_{1g}} = -13.856, \Theta^{2211}_{E_gE_gT_{1g}T_{1g}} = 12.0, \Theta^{2222}_{E_gE_gT_{1g}T_{1g}} = 12.0$
45	$\Theta^{1221}_{T_{1g}T_{2g}T_{1u}T_{2u}} = 8.0, \Theta^{1251}_{T_{1g}T_{2g}T_{1u}T_{2u}} = 5.842, \Theta^{1322}_{T_{1g}T_{2g}T_{1u}T_{2u}} = 8.0, \Theta^{1352}_{T_{1g}T_{2g}T_{1u}T_{2u}} = 5.842, \Theta^{2133}_{T_{1g}T_{2g}T_{1u}T_{2u}} = -8.0, \Theta^{2163}_{T_{1g}T_{2g}T_{1u}T_{2u}} = -5.842, \Theta^{2332}_{T_{1g}T_{2g}T_{1u}T_{2u}} = 8.0, \Theta^{2362}_{T_{1g}T_{2g}T_{1u}T_{2u}} = 5.842, \Theta^{3113}_{T_{1g}T_{2g}T_{1u}T_{2u}} = 8.0, \Theta^{3143}_{T_{1g}T_{2g}T_{1u}T_{2u}} = 5.842, \Theta^{3211}_{T_{1g}T_{2g}T_{1u}T_{2u}} = -8.0, \Theta^{3241}_{T_{1g}T_{2g}T_{1u}T_{2u}} = -5.842$

46	$\Theta^{1233}_{T_{1g}T_{2g}T_{1u}T_{2u}} = -5.842, \Theta^{1263}_{T_{1g}T_{2g}T_{1u}T_{2u}} = -8.0, \Theta^{1313}_{T_{1g}T_{2g}T_{1u}T_{2u}} = 5.842, \Theta^{1343}_{T_{1g}T_{2g}T_{1u}T_{2u}} = 8.0, \Theta^{2121}_{T_{1g}T_{2g}T_{1u}T_{2u}} = 5.842, \Theta^{2151}_{T_{1g}T_{2g}T_{1u}T_{2u}} = 8.0, \Theta^{2311}_{T_{1g}T_{2g}T_{1u}T_{2u}} = -5.842, \Theta^{2341}_{T_{1g}T_{2g}T_{1u}T_{2u}} = -8.0, \Theta^{3122}_{T_{1g}T_{2g}T_{1u}T_{2u}} = 5.842, \Theta^{3152}_{T_{1g}T_{2g}T_{1u}T_{2u}} = 8.0, \Theta^{3232}_{T_{1g}T_{2g}T_{1u}T_{2u}} = 5.842, \Theta^{3262}_{T_{1g}T_{2g}T_{1u}T_{2u}} = 8.0$
47	$\Theta^{1111}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 16.0, \Theta^{1114}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 46.739, \Theta^{1144}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 51.2, \Theta^{1444}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 24.927, \Theta^{2222}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 16.0, \Theta^{2225}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 46.739, \Theta^{2255}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 51.2, \Theta^{2555}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 24.927, \Theta^{3333}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 16.0, \Theta^{3336}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 46.739, \Theta^{3366}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 51.2, \Theta^{3666}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 24.927, \Theta^{4444}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 4.551, \Theta^{5555}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 4.551, \Theta^{6666}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 4.551$
48	$\Theta^{1123}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -3.116, \Theta^{1131}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -3.116, \Theta^{1153}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -4.267, \Theta^{1161}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -4.267, \Theta^{1222}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 3.116, \Theta^{1243}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -8.533, \Theta^{1252}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 8.533, \Theta^{1332}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -3.116, \Theta^{1341}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -8.533, \Theta^{1362}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -8.533, \Theta^{1453}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -11.685, \Theta^{1461}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -11.685, \Theta^{1552}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 5.842, \Theta^{1662}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -5.842, \Theta^{2231}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 3.116, \Theta^{2242}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 4.267, \Theta^{2261}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 4.267, \Theta^{2333}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 3.116, \Theta^{2351}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 8.533, \Theta^{2363}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 8.533, \Theta^{2443}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -5.842, \Theta^{2452}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 11.685, \Theta^{2561}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 11.685, \Theta^{2663}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 5.842, \Theta^{3342}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -4.267, \Theta^{3353}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 4.267, \Theta^{3441}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -5.842, \Theta^{3462}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -11.685, \Theta^{3551}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 5.842, \Theta^{3563}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 11.685, \Theta^{4453}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -8.0, \Theta^{4461}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -8.0, \Theta^{4552}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 8.0, \Theta^{4662}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -8.0, \Theta^{5561}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 8.0, \Theta^{5663}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 8.0$
49	$\Theta^{1113}_{E_gT_{2g}T_{1u}T_{1u}} = 2.921, \Theta^{1116}_{E_gT_{2g}T_{1u}T_{1u}} = 0.267, \Theta^{1134}_{E_gT_{2g}T_{1u}T_{1u}} = 5.867, \Theta^{1146}_{E_gT_{2g}T_{1u}T_{1u}} = 2.921, \Theta^{1212}_{E_gT_{2g}T_{1u}T_{1u}} = 2.921, \Theta^{1215}_{E_gT_{2g}T_{1u}T_{1u}} = 0.267, \Theta^{1224}_{E_gT_{2g}T_{1u}T_{1u}} = 5.867, \Theta^{1245}_{E_gT_{2g}T_{1u}T_{1u}} = 2.921, \Theta^{1323}_{E_gT_{2g}T_{1u}T_{1u}} = 5.842, \Theta^{1326}_{E_gT_{2g}T_{1u}T_{1u}} = 6.133, \Theta^{1335}_{E_gT_{2g}T_{1u}T_{1u}} = 6.133, \Theta^{1356}_{E_gT_{2g}T_{1u}T_{1u}} = 5.842, \Theta^{2113}_{E_gT_{2g}T_{1u}T_{1u}} = 5.06, \Theta^{2116}_{E_gT_{2g}T_{1u}T_{1u}} = 6.928, \Theta^{2134}_{E_gT_{2g}T_{1u}T_{1u}} = 3.695, \Theta^{2146}_{E_gT_{2g}T_{1u}T_{1u}} = 5.06, \Theta^{2212}_{E_gT_{2g}T_{1u}T_{1u}} = -5.06, \Theta^{2215}_{E_gT_{2g}T_{1u}T_{1u}} = -6.928, \Theta^{2224}_{E_gT_{2g}T_{1u}T_{1u}} = -3.695, \Theta^{2245}_{E_gT_{2g}T_{1u}T_{1u}} = -5.06, \Theta^{2326}_{E_gT_{2g}T_{1u}T_{1u}} = -3.233, \Theta^{2335}_{E_gT_{2g}T_{1u}T_{1u}} = 3.233$
50	$\Theta^{1111}_{A_{1g}E_gT_{1u}T_{1u}} = 10.119, \Theta^{1114}_{A_{1g}E_gT_{1u}T_{1u}} = 21.246, \Theta^{1122}_{A_{1g}E_gT_{1u}T_{1u}} = -5.06, \Theta^{1125}_{A_{1g}E_gT_{1u}T_{1u}} = -10.623, \Theta^{1133}_{A_{1g}E_gT_{1u}T_{1u}} = -5.06, \Theta^{1136}_{A_{1g}E_gT_{1u}T_{1u}} = -10.623, \Theta^{1144}_{A_{1g}E_gT_{1u}T_{1u}} = 10.119, \Theta^{1155}_{A_{1g}E_gT_{1u}T_{1u}} = -5.06, \Theta^{1166}_{A_{1g}E_gT_{1u}T_{1u}} = -5.06, \Theta^{1222}_{A_{1g}E_gT_{1u}T_{1u}} = -8.764, \Theta^{1225}_{A_{1g}E_gT_{1u}T_{1u}} = -18.4, \Theta^{1233}_{A_{1g}E_gT_{1u}T_{1u}} = 8.764, \Theta^{1236}_{A_{1g}E_gT_{1u}T_{1u}} = 18.4, \Theta^{1255}_{A_{1g}E_gT_{1u}T_{1u}} = -8.764, \Theta^{1266}_{A_{1g}E_gT_{1u}T_{1u}} = 8.764$

51	$\Theta^{1122}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 8.533, \Theta^{1125}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 23.369, \Theta^{1155}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 16.0, \Theta^{2233}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 8.533, \Theta^{2236}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 23.369, \Theta^{2266}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 16.0, \Theta^{3311}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 8.533, \Theta^{3314}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 23.369, \Theta^{3344}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 16.0$
52	$\Theta^{1111}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 5.842, \Theta^{1133}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 5.842, \Theta^{1411}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 12.267, \Theta^{1433}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 12.267, \Theta^{2211}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 5.842, \Theta^{2222}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 5.842, \Theta^{2511}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 12.267, \Theta^{2522}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 12.267, \Theta^{3322}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 5.842, \Theta^{3333}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 5.842, \Theta^{3622}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 12.267, \Theta^{3633}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 12.267, \Theta^{4411}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 5.842, \Theta^{4433}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 5.842, \Theta^{5511}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 5.842, \Theta^{5522}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 5.842, \Theta^{6622}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 5.842, \Theta^{6633}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 5.842$
53	$\Theta^{1111}_{A_{1g}A_{1g}T_{1u}T_{1u}} = 16.0, \Theta^{1114}_{A_{1g}A_{1g}T_{1u}T_{1u}} = 23.369, \Theta^{1122}_{A_{1g}A_{1g}T_{1u}T_{1u}} = 16.0, \Theta^{1125}_{A_{1g}A_{1g}T_{1u}T_{1u}} = 23.369, \Theta^{1133}_{A_{1g}A_{1g}T_{1u}T_{1u}} = 16.0, \Theta^{1136}_{A_{1g}A_{1g}T_{1u}T_{1u}} = 23.369, \Theta^{1144}_{A_{1g}A_{1g}T_{1u}T_{1u}} = 8.533, \Theta^{1155}_{A_{1g}A_{1g}T_{1u}T_{1u}} = 8.533, \Theta^{1166}_{A_{1g}A_{1g}T_{1u}T_{1u}} = 8.533$
54	$\Theta^{1122}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 4.551, \Theta^{1125}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 12.464, \Theta^{1133}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 4.551, \Theta^{1136}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 12.464, \Theta^{1155}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 8.533, \Theta^{1166}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 8.533, \Theta^{1224}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 12.464, \Theta^{1245}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 34.133, \Theta^{1334}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 12.464, \Theta^{1346}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 34.133, \Theta^{1455}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 23.369, \Theta^{1466}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 23.369, \Theta^{2233}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 4.551, \Theta^{2236}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 12.464, \Theta^{2244}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 8.533, \Theta^{2266}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 8.533, \Theta^{2335}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 12.464, \Theta^{2356}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 34.133, \Theta^{2445}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 23.369, \Theta^{2566}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 23.369, \Theta^{3344}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 8.533, \Theta^{3355}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 8.533, \Theta^{3446}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 23.369, \Theta^{3556}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 23.369, \Theta^{4455}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 16.0, \Theta^{4466}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 16.0, \Theta^{5566}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 16.0$
55	$\Theta^{1123}_{T_{1g}T_{2g}T_{1u}T_{2u}} = 11.685, \Theta^{1153}_{T_{1g}T_{2g}T_{1u}T_{2u}} = 16.0, \Theta^{2231}_{T_{1g}T_{2g}T_{1u}T_{2u}} = -11.685, \Theta^{2261}_{T_{1g}T_{2g}T_{1u}T_{2u}} = -16.0, \Theta^{3312}_{T_{1g}T_{2g}T_{1u}T_{2u}} = 11.685, \Theta^{3342}_{T_{1g}T_{2g}T_{1u}T_{2u}} = 16.0$
56	$\Theta^{1123}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 4.267, \Theta^{1131}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 4.267, \Theta^{1153}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 3.116, \Theta^{1161}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 3.116, \Theta^{1222}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -4.267, \Theta^{1243}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 11.685, \Theta^{1252}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -11.685, \Theta^{1332}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 4.267, \Theta^{1341}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 11.685, \Theta^{1362}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 11.685, \Theta^{1453}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 8.533, \Theta^{1461}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 8.533, \Theta^{1552}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -8.0, \Theta^{1662}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 8.0, \Theta^{2231}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -4.267, \Theta^{2242}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -3.116, \Theta^{2261}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -3.116, \Theta^{2333}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -4.267, \Theta^{2351}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -11.685, \Theta^{2363}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -11.685, \Theta^{2443}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 8.0, \Theta^{2452}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -8.533, \Theta^{2561}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -8.533, \Theta^{2663}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -8.0, \Theta^{3342}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 3.116, \Theta^{3353}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -3.116, \Theta^{3441}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 8.0, \Theta^{3462}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 8.533, \Theta^{3551}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -8.0, \Theta^{3563}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -8.533, \Theta^{4453}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 5.842, \Theta^{4461}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 5.842, \Theta^{4552}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -5.842, \Theta^{4662}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 5.842, \Theta^{5561}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -5.842, \Theta^{5663}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -5.842$

57	$\Theta^{1113}_{E_gT_{1g}T_{1u}T_{1u}} = 8.764, \Theta^{1116}_{E_gT_{1g}T_{1u}T_{1u}} = 8.267, \Theta^{1134}_{E_gT_{1g}T_{1u}T_{1u}} = 10.133, \Theta^{1146}_{E_gT_{1g}T_{1u}T_{1u}} = 8.764, \Theta^{1212}_{E_gT_{1g}T_{1u}T_{1u}} = -8.764, \Theta^{1215}_{E_gT_{1g}T_{1u}T_{1u}} = -8.267, \Theta^{1224}_{E_gT_{1g}T_{1u}T_{1u}} = -10.133, \Theta^{1245}_{E_gT_{1g}T_{1u}T_{1u}} = -8.764, \Theta^{1326}_{E_gT_{1g}T_{1u}T_{1u}} = 1.867, \Theta^{1335}_{E_gT_{1g}T_{1u}T_{1u}} = -1.867, \Theta^{2113}_{E_gT_{1g}T_{1u}T_{1u}} = -5.06, \Theta^{2116}_{E_gT_{1g}T_{1u}T_{1u}} = -6.928, \Theta^{2134}_{E_gT_{1g}T_{1u}T_{1u}} = -3.695, \Theta^{2146}_{E_gT_{1g}T_{1u}T_{1u}} = -5.06, \Theta^{2212}_{E_gT_{1g}T_{1u}T_{1u}} = -5.06, \Theta^{2215}_{E_gT_{1g}T_{1u}T_{1u}} = -6.928, \Theta^{2224}_{E_gT_{1g}T_{1u}T_{1u}} = -3.695, \Theta^{2245}_{E_gT_{1g}T_{1u}T_{1u}} = -5.06, \Theta^{2323}_{E_gT_{1g}T_{1u}T_{1u}} = -10.119, \Theta^{2326}_{E_gT_{1g}T_{1u}T_{1u}} = -10.623, \Theta^{2335}_{E_gT_{1g}T_{1u}T_{1u}} = -10.623, \Theta^{2356}_{E_gT_{1g}T_{1u}T_{1u}} = -10.119$
58	$\Theta^{1123}_{A_{1g}T_{1g}T_{1g}T_{2g}} = 16.0, \Theta^{1132}_{A_{1g}T_{1g}T_{1g}T_{2g}} = 16.0, \Theta^{1231}_{A_{1g}T_{1g}T_{1g}T_{2g}} = 16.0$
59	$\Theta^{1223}_{T_{2g}T_{2g}T_{1u}T_{1u}} = -11.685, \Theta^{1226}_{T_{2g}T_{2g}T_{1u}T_{1u}} = -12.267, \Theta^{1235}_{T_{2g}T_{2g}T_{1u}T_{1u}} = -12.267, \Theta^{1256}_{T_{2g}T_{2g}T_{1u}T_{1u}} = -11.685, \Theta^{1312}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 11.685, \Theta^{1315}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 12.267, \Theta^{1324}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 12.267, \Theta^{1345}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 11.685, \Theta^{2313}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 11.685, \Theta^{2316}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 12.267, \Theta^{2334}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 12.267, \Theta^{2346}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 11.685$
60	$\Theta^{1123}_{E_gE_gT_{1u}T_{2u}} = 6.0, \Theta^{1131}_{E_gE_gT_{1u}T_{2u}} = 6.0, \Theta^{1153}_{E_gE_gT_{1u}T_{2u}} = 4.382, \Theta^{1161}_{E_gE_gT_{1u}T_{2u}} = 4.382, \Theta^{1212}_{E_gE_gT_{1u}T_{2u}} = -13.856, \Theta^{1223}_{E_gE_gT_{1u}T_{2u}} = 6.928, \Theta^{1231}_{E_gE_gT_{1u}T_{2u}} = -6.928, \Theta^{1242}_{E_gE_gT_{1u}T_{2u}} = -10.119, \Theta^{1253}_{E_gE_gT_{1u}T_{2u}} = 5.06, \Theta^{1261}_{E_gE_gT_{1u}T_{2u}} = -5.06, \Theta^{2223}_{E_gE_gT_{1u}T_{2u}} = -6.0, \Theta^{2231}_{E_gE_gT_{1u}T_{2u}} = -6.0, \Theta^{2253}_{E_gE_gT_{1u}T_{2u}} = -4.382, \Theta^{2261}_{E_gE_gT_{1u}T_{2u}} = -4.382$
61	$\Theta^{1113}_{E_gT_{1g}T_{1u}T_{1u}} = -10.119, \Theta^{1116}_{E_gT_{1g}T_{1u}T_{1u}} = -10.623, \Theta^{1134}_{E_gT_{1g}T_{1u}T_{1u}} = -10.623, \Theta^{1146}_{E_gT_{1g}T_{1u}T_{1u}} = -10.119, \Theta^{1212}_{E_gT_{1g}T_{1u}T_{1u}} = 10.119, \Theta^{1215}_{E_gT_{1g}T_{1u}T_{1u}} = 10.623, \Theta^{1224}_{E_gT_{1g}T_{1u}T_{1u}} = 10.623, \Theta^{1245}_{E_gT_{1g}T_{1u}T_{1u}} = 10.119, \Theta^{2113}_{E_gT_{1g}T_{1u}T_{1u}} = 5.842, \Theta^{2116}_{E_gT_{1g}T_{1u}T_{1u}} = 6.133, \Theta^{2134}_{E_gT_{1g}T_{1u}T_{1u}} = 6.133, \Theta^{2146}_{E_gT_{1g}T_{1u}T_{1u}} = 5.842, \Theta^{2212}_{E_gT_{1g}T_{1u}T_{1u}} = 5.842, \Theta^{2215}_{E_gT_{1g}T_{1u}T_{1u}} = 6.133, \Theta^{2224}_{E_gT_{1g}T_{1u}T_{1u}} = 6.133, \Theta^{2245}_{E_gT_{1g}T_{1u}T_{1u}} = 5.842, \Theta^{2323}_{E_gT_{1g}T_{1u}T_{1u}} = 11.685, \Theta^{2326}_{E_gT_{1g}T_{1u}T_{1u}} = 12.267, \Theta^{2335}_{E_gT_{1g}T_{1u}T_{1u}} = 12.267, \Theta^{2356}_{E_gT_{1g}T_{1u}T_{1u}} = 11.685$

62	$\Theta^{1123}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -4.267, \Theta^{1131}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -4.267, \Theta^{1153}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -5.842, \Theta^{1161}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -5.842, \Theta^{1222}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 4.267, \Theta^{1243}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -8.958, \Theta^{1252}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 8.958, \Theta^{1332}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -4.267, \Theta^{1341}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -8.958, \Theta^{1362}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -8.958, \Theta^{1453}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -12.267, \Theta^{1461}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -12.267, \Theta^{1552}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 4.267, \Theta^{1662}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -4.267, \Theta^{2231}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 4.267, \Theta^{2242}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 5.842, \Theta^{2261}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 5.842, \Theta^{2333}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 4.267, \Theta^{2351}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 8.958, \Theta^{2363}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 8.958, \Theta^{2443}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -4.267, \Theta^{2452}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 12.267, \Theta^{2561}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 12.267, \Theta^{2663}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 4.267, \Theta^{3342}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -5.842, \Theta^{3353}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 5.842, \Theta^{3441}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -4.267, \Theta^{3462}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -12.267, \Theta^{3551}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 4.267, \Theta^{3563}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 12.267, \Theta^{4453}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -5.842, \Theta^{4461}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -5.842, \Theta^{4552}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 5.842, \Theta^{4662}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -5.842, \Theta^{5561}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 5.842, \Theta^{5663}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 5.842$
63	$\Theta^{1123}_{E_gT_{1g}T_{1g}T_{2g}} = 13.856, \Theta^{1132}_{E_gT_{1g}T_{1g}T_{2g}} = -6.928, \Theta^{1231}_{E_gT_{1g}T_{1g}T_{2g}} = -6.928, \Theta^{2132}_{E_gT_{1g}T_{1g}T_{2g}} = 12.0, \Theta^{2231}_{E_gT_{1g}T_{1g}T_{2g}} = -12.0$
64	$\Theta^{1112}_{T_{1u}T_{2u}T_{2u}T_{2u}} = 5.842, \Theta^{1233}_{T_{1u}T_{2u}T_{2u}T_{2u}} = -5.842, \Theta^{2113}_{T_{1u}T_{2u}T_{2u}T_{2u}} = -5.842, \Theta^{2223}_{T_{1u}T_{2u}T_{2u}T_{2u}} = 5.842, \Theta^{3122}_{T_{1u}T_{2u}T_{2u}T_{2u}} = 5.842, \Theta^{3133}_{T_{1u}T_{2u}T_{2u}T_{2u}} = -5.842, \Theta^{4112}_{T_{1u}T_{2u}T_{2u}T_{2u}} = 8.0, \Theta^{4233}_{T_{1u}T_{2u}T_{2u}T_{2u}} = -8.0, \Theta^{5113}_{T_{1u}T_{2u}T_{2u}T_{2u}} = -8.0, \Theta^{5223}_{T_{1u}T_{2u}T_{2u}T_{2u}} = 8.0, \Theta^{6122}_{T_{1u}T_{2u}T_{2u}T_{2u}} = 8.0, \Theta^{6133}_{T_{1u}T_{2u}T_{2u}T_{2u}} = -8.0$
65	$\Theta^{1111}_{E_gE_gT_{1g}T_{2g}} = 3.464, \Theta^{1122}_{E_gE_gT_{1g}T_{2g}} = -3.464, \Theta^{1211}_{E_gE_gT_{1g}T_{2g}} = 4.0, \Theta^{1222}_{E_gE_gT_{1g}T_{2g}} = 4.0, \Theta^{1233}_{E_gE_gT_{1g}T_{2g}} = -8.0, \Theta^{2211}_{E_gE_gT_{1g}T_{2g}} = -3.464, \Theta^{2222}_{E_gE_gT_{1g}T_{2g}} = 3.464$
66	$\Theta^{1111}_{E_gE_gT_{2u}T_{2u}} = -3.464, \Theta^{1122}_{E_gE_gT_{2u}T_{2u}} = 6.928, \Theta^{1133}_{E_gE_gT_{2u}T_{2u}} = -3.464, \Theta^{1211}_{E_gE_gT_{2u}T_{2u}} = -12.0, \Theta^{1233}_{E_gE_gT_{2u}T_{2u}} = 12.0, \Theta^{2211}_{E_gE_gT_{2u}T_{2u}} = 3.464, \Theta^{2222}_{E_gE_gT_{2u}T_{2u}} = -6.928, \Theta^{2233}_{E_gE_gT_{2u}T_{2u}} = 3.464$
67	$\Theta^{1111}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -5.842, \Theta^{1114}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -12.267, \Theta^{1133}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 5.842, \Theta^{1136}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 12.267, \Theta^{1144}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -5.842, \Theta^{1166}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 5.842, \Theta^{2211}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 5.842, \Theta^{2214}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 12.267, \Theta^{2222}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -5.842, \Theta^{2225}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -12.267, \Theta^{2244}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 5.842, \Theta^{2255}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -5.842, \Theta^{3322}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 5.842, \Theta^{3325}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 12.267, \Theta^{3333}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -5.842, \Theta^{3336}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -12.267, \Theta^{3355}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 5.842, \Theta^{3366}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -5.842$
68	$\Theta^{1122}_{T_{1g}T_{1g}T_{2g}T_{2g}} = 8.0, \Theta^{1133}_{T_{1g}T_{1g}T_{2g}T_{2g}} = 8.0, \Theta^{2211}_{T_{1g}T_{1g}T_{2g}T_{2g}} = 8.0, \Theta^{2233}_{T_{1g}T_{1g}T_{2g}T_{2g}} = 8.0, \Theta^{3311}_{T_{1g}T_{1g}T_{2g}T_{2g}} = 8.0, \Theta^{3322}_{T_{1g}T_{1g}T_{2g}T_{2g}} = 8.0$
69	$\Theta^{1133}_{T_{2g}T_{2g}T_{2u}T_{2u}} = 16.0, \Theta^{2211}_{T_{2g}T_{2g}T_{2u}T_{2u}} = 16.0, \Theta^{3322}_{T_{2g}T_{2g}T_{2u}T_{2u}} = 16.0$

70	$\Theta^{1223}_{T_{1u}T_{1u}T_{2u}T_{2u}} = -8.533, \Theta^{1312}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 8.533, \Theta^{1523}_{T_{1u}T_{1u}T_{2u}T_{2u}} = -11.685, \Theta^{1612}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 11.685, \Theta^{2313}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 8.533, \Theta^{2423}_{T_{1u}T_{1u}T_{2u}T_{2u}} = -11.685, \Theta^{2613}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 11.685, \Theta^{3412}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 11.685, \Theta^{3513}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 11.685, \Theta^{4523}_{T_{1u}T_{1u}T_{2u}T_{2u}} = -16.0, \Theta^{4612}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 16.0, \Theta^{5613}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 16.0$
71	$\Theta^{1112}_{T_{2g}T_{2g}T_{1u}T_{2u}} = -8.0, \Theta^{1131}_{T_{2g}T_{2g}T_{1u}T_{2u}} = -8.0, \Theta^{1142}_{T_{2g}T_{2g}T_{1u}T_{2u}} = -5.842, \Theta^{1161}_{T_{2g}T_{2g}T_{1u}T_{2u}} = -5.842, \Theta^{2212}_{T_{2g}T_{2g}T_{1u}T_{2u}} = 8.0, \Theta^{2223}_{T_{2g}T_{2g}T_{1u}T_{2u}} = -8.0, \Theta^{2242}_{T_{2g}T_{2g}T_{1u}T_{2u}} = 5.842, \Theta^{2253}_{T_{2g}T_{2g}T_{1u}T_{2u}} = -5.842, \Theta^{3323}_{T_{2g}T_{2g}T_{1u}T_{2u}} = 8.0, \Theta^{3331}_{T_{2g}T_{2g}T_{1u}T_{2u}} = 8.0, \Theta^{3353}_{T_{2g}T_{2g}T_{1u}T_{2u}} = 5.842, \Theta^{3361}_{T_{2g}T_{2g}T_{1u}T_{2u}} = 5.842$
72	$\Theta^{1123}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -5.842, \Theta^{1131}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -5.842, \Theta^{1153}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -8.0, \Theta^{1161}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -8.0, \Theta^{1222}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 5.842, \Theta^{1243}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -8.533, \Theta^{1252}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 8.533, \Theta^{1332}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -5.842, \Theta^{1341}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -8.533, \Theta^{1362}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -8.533, \Theta^{1453}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -11.685, \Theta^{1461}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -11.685, \Theta^{1552}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 3.116, \Theta^{1662}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -3.116, \Theta^{2231}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 5.842, \Theta^{2242}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 8.0, \Theta^{2261}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 8.0, \Theta^{2333}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 5.842, \Theta^{2351}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 8.533, \Theta^{2363}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 8.533, \Theta^{2443}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -3.116, \Theta^{2452}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 11.685, \Theta^{2561}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 11.685, \Theta^{2663}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 3.116, \Theta^{3342}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -8.0, \Theta^{3353}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 8.0, \Theta^{3441}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -3.116, \Theta^{3462}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -11.685, \Theta^{3551}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 3.116, \Theta^{3563}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 11.685, \Theta^{4453}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -4.267, \Theta^{4461}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -4.267, \Theta^{4552}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 4.267, \Theta^{4662}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -4.267, \Theta^{5561}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 4.267, \Theta^{5663}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 4.267$
73	$\Theta^{1223}_{T_{1g}T_{1g}T_{1u}T_{1u}} = -8.533, \Theta^{1226}_{T_{1g}T_{1g}T_{1u}T_{1u}} = -11.685, \Theta^{1235}_{T_{1g}T_{1g}T_{1u}T_{1u}} = -11.685, \Theta^{1256}_{T_{1g}T_{1g}T_{1u}T_{1u}} = -16.0, \Theta^{1312}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 8.533, \Theta^{1315}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 11.685, \Theta^{1324}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 11.685, \Theta^{1345}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 16.0, \Theta^{2313}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 8.533, \Theta^{2316}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 11.685, \Theta^{2334}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 11.685, \Theta^{2346}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 16.0$
74	$\Theta^{1221}_{T_{1g}T_{1g}T_{1u}T_{2u}} = 5.842, \Theta^{1233}_{T_{1g}T_{1g}T_{1u}T_{2u}} = 5.842, \Theta^{1251}_{T_{1g}T_{1g}T_{1u}T_{2u}} = 8.0, \Theta^{1263}_{T_{1g}T_{1g}T_{1u}T_{2u}} = 8.0, \Theta^{1313}_{T_{1g}T_{1g}T_{1u}T_{2u}} = 5.842, \Theta^{1322}_{T_{1g}T_{1g}T_{1u}T_{2u}} = -5.842, \Theta^{1343}_{T_{1g}T_{1g}T_{1u}T_{2u}} = 8.0, \Theta^{1352}_{T_{1g}T_{1g}T_{1u}T_{2u}} = -8.0, \Theta^{2311}_{T_{1g}T_{1g}T_{1u}T_{2u}} = 5.842, \Theta^{2332}_{T_{1g}T_{1g}T_{1u}T_{2u}} = 5.842, \Theta^{2341}_{T_{1g}T_{1g}T_{1u}T_{2u}} = 8.0, \Theta^{2362}_{T_{1g}T_{1g}T_{1u}T_{2u}} = 8.0$

75	$\Theta^{1123}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 8.0, \Theta^{1131}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 8.0, \Theta^{1153}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 5.842, \Theta^{1161}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 5.842, \Theta^{1222}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -8.0, \Theta^{1243}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 11.685, \Theta^{1252}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -11.685, \Theta^{1332}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 8.0, \Theta^{1341}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 11.685, \Theta^{1362}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 11.685, \Theta^{1453}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 8.533, \Theta^{1461}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 8.533, \Theta^{1552}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -4.267, \Theta^{1662}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 4.267, \Theta^{2231}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -8.0, \Theta^{2242}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -5.842, \Theta^{2261}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -5.842, \Theta^{2333}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -8.0, \Theta^{2351}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -11.685, \Theta^{2363}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -11.685, \Theta^{2443}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 4.267, \Theta^{2452}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -8.533, \Theta^{2561}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -8.533, \Theta^{2663}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -4.267, \Theta^{3342}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 5.842, \Theta^{3353}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -5.842, \Theta^{3441}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 4.267, \Theta^{3462}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 8.533, \Theta^{3551}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -4.267, \Theta^{3563}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -8.533, \Theta^{4453}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 3.116, \Theta^{4461}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 3.116, \Theta^{4552}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -3.116, \Theta^{4662}_{T_{1u}T_{1u}T_{1u}T_{2u}} = 3.116, \Theta^{5561}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -3.116, \Theta^{5663}_{T_{1u}T_{1u}T_{1u}T_{2u}} = -3.116$
76	$\Theta^{1221}_{T_{1g}T_{2g}T_{1u}T_{2u}} = -5.842, \Theta^{1251}_{T_{1g}T_{2g}T_{1u}T_{2u}} = -8.0, \Theta^{1322}_{T_{1g}T_{2g}T_{1u}T_{2u}} = -5.842, \Theta^{1352}_{T_{1g}T_{2g}T_{1u}T_{2u}} = -8.0, \Theta^{2133}_{T_{1g}T_{2g}T_{1u}T_{2u}} = 5.842, \Theta^{2163}_{T_{1g}T_{2g}T_{1u}T_{2u}} = 8.0, \Theta^{2332}_{T_{1g}T_{2g}T_{1u}T_{2u}} = -5.842, \Theta^{2362}_{T_{1g}T_{2g}T_{1u}T_{2u}} = -8.0, \Theta^{3113}_{T_{1g}T_{2g}T_{1u}T_{2u}} = -5.842, \Theta^{3143}_{T_{1g}T_{2g}T_{1u}T_{2u}} = -8.0, \Theta^{3211}_{T_{1g}T_{2g}T_{1u}T_{2u}} = 5.842, \Theta^{3241}_{T_{1g}T_{2g}T_{1u}T_{2u}} = 8.0$
77	$\Theta^{1112}_{T_{1g}T_{1g}T_{1u}T_{2u}} = -8.0, \Theta^{1131}_{T_{1g}T_{1g}T_{1u}T_{2u}} = -8.0, \Theta^{1142}_{T_{1g}T_{1g}T_{1u}T_{2u}} = -5.842, \Theta^{1161}_{T_{1g}T_{1g}T_{1u}T_{2u}} = -5.842, \Theta^{2212}_{T_{1g}T_{1g}T_{1u}T_{2u}} = 8.0, \Theta^{2223}_{T_{1g}T_{1g}T_{1u}T_{2u}} = -8.0, \Theta^{2242}_{T_{1g}T_{1g}T_{1u}T_{2u}} = 5.842, \Theta^{2253}_{T_{1g}T_{1g}T_{1u}T_{2u}} = -5.842, \Theta^{3323}_{T_{1g}T_{1g}T_{1u}T_{2u}} = 8.0, \Theta^{3331}_{T_{1g}T_{1g}T_{1u}T_{2u}} = 8.0, \Theta^{3353}_{T_{1g}T_{1g}T_{1u}T_{2u}} = 5.842, \Theta^{3361}_{T_{1g}T_{1g}T_{1u}T_{2u}} = 5.842$
78	$\Theta^{1113}_{E_gT_{1g}T_{1u}T_{1u}} = -6.928, \Theta^{1116}_{E_gT_{1g}T_{1u}T_{1u}} = -5.06, \Theta^{1134}_{E_gT_{1g}T_{1u}T_{1u}} = -5.06, \Theta^{1146}_{E_gT_{1g}T_{1u}T_{1u}} = -3.695, \Theta^{1212}_{E_gT_{1g}T_{1u}T_{1u}} = 6.928, \Theta^{1215}_{E_gT_{1g}T_{1u}T_{1u}} = 5.06, \Theta^{1224}_{E_gT_{1g}T_{1u}T_{1u}} = 5.06, \Theta^{1245}_{E_gT_{1g}T_{1u}T_{1u}} = 3.695, \Theta^{2113}_{E_gT_{1g}T_{1u}T_{1u}} = 4.0, \Theta^{2116}_{E_gT_{1g}T_{1u}T_{1u}} = 2.921, \Theta^{2134}_{E_gT_{1g}T_{1u}T_{1u}} = 2.921, \Theta^{2146}_{E_gT_{1g}T_{1u}T_{1u}} = 2.133, \Theta^{2212}_{E_gT_{1g}T_{1u}T_{1u}} = 4.0, \Theta^{2215}_{E_gT_{1g}T_{1u}T_{1u}} = 2.921, \Theta^{2224}_{E_gT_{1g}T_{1u}T_{1u}} = 2.921, \Theta^{2245}_{E_gT_{1g}T_{1u}T_{1u}} = 2.133, \Theta^{2323}_{E_gT_{1g}T_{1u}T_{1u}} = 8.0, \Theta^{2326}_{E_gT_{1g}T_{1u}T_{1u}} = 5.842, \Theta^{2335}_{E_gT_{1g}T_{1u}T_{1u}} = 5.842, \Theta^{2356}_{E_gT_{1g}T_{1u}T_{1u}} = 4.267$
79	$\Theta^{1122}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 11.685, \Theta^{1125}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 20.8, \Theta^{1133}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 11.685, \Theta^{1136}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 20.8, \Theta^{1155}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 8.958, \Theta^{1166}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 8.958, \Theta^{1224}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 20.8, \Theta^{1245}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 35.833, \Theta^{1334}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 20.8, \Theta^{1346}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 35.833, \Theta^{1455}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 15.076, \Theta^{1466}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 15.076, \Theta^{2233}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 11.685, \Theta^{2236}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 20.8, \Theta^{2244}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 8.958, \Theta^{2266}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 8.958, \Theta^{2335}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 20.8, \Theta^{2356}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 35.833, \Theta^{2445}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 15.076, \Theta^{2566}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 15.076, \Theta^{3344}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 8.958, \Theta^{3355}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 8.958, \Theta^{3446}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 15.076, \Theta^{3556}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 15.076, \Theta^{4455}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 6.232, \Theta^{4466}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 6.232, \Theta^{5566}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 6.232$

80	$\Theta^{1111}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 8.0, \Theta^{1133}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 8.0, \Theta^{1411}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 11.685, \Theta^{1433}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 11.685, \Theta^{2211}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 8.0, \Theta^{2222}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 8.0, \Theta^{2511}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 11.685, \Theta^{2522}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 11.685, \Theta^{3322}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 8.0, \Theta^{3333}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 8.0, \Theta^{3622}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 11.685, \Theta^{3633}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 11.685, \Theta^{4411}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 4.267, \Theta^{4433}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 4.267, \Theta^{5511}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 4.267, \Theta^{5522}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 4.267, \Theta^{6622}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 4.267, \Theta^{6633}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 4.267$
81	$\Theta^{1123}_{E_gE_gT_{1u}T_{2u}} = -5.06, \Theta^{1131}_{E_gE_gT_{1u}T_{2u}} = -5.06, \Theta^{1153}_{E_gE_gT_{1u}T_{2u}} = -6.928, \Theta^{1161}_{E_gE_gT_{1u}T_{2u}} = -6.928, \Theta^{1212}_{E_gE_gT_{1u}T_{2u}} = 11.685, \Theta^{1223}_{E_gE_gT_{1u}T_{2u}} = -5.842, \Theta^{1231}_{E_gE_gT_{1u}T_{2u}} = 5.842, \Theta^{1242}_{E_gE_gT_{1u}T_{2u}} = 16.0, \Theta^{1253}_{E_gE_gT_{1u}T_{2u}} = -8.0, \Theta^{1261}_{E_gE_gT_{1u}T_{2u}} = 8.0, \Theta^{2223}_{E_gE_gT_{1u}T_{2u}} = 5.06, \Theta^{2231}_{E_gE_gT_{1u}T_{2u}} = 5.06, \Theta^{2253}_{E_gE_gT_{1u}T_{2u}} = 6.928, \Theta^{2261}_{E_gE_gT_{1u}T_{2u}} = 6.928$
82	$\Theta^{1111}_{T_{1g}T_{1g}T_{2g}T_{2g}} = 16.0, \Theta^{2222}_{T_{1g}T_{1g}T_{2g}T_{2g}} = 16.0, \Theta^{3333}_{T_{1g}T_{1g}T_{2g}T_{2g}} = 16.0$
83	$\Theta^{1213}_{T_{1g}T_{2g}T_{2u}T_{2u}} = 8.0, \Theta^{1323}_{T_{1g}T_{2g}T_{2u}T_{2u}} = -8.0, \Theta^{2113}_{T_{1g}T_{2g}T_{2u}T_{2u}} = -8.0, \Theta^{2312}_{T_{1g}T_{2g}T_{2u}T_{2u}} = -8.0, \Theta^{3123}_{T_{1g}T_{2g}T_{2u}T_{2u}} = 8.0, \Theta^{3212}_{T_{1g}T_{2g}T_{2u}T_{2u}} = 8.0$
84	$\Theta^{1122}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 11.685, \Theta^{1125}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 24.533, \Theta^{1155}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 11.685, \Theta^{2233}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 11.685, \Theta^{2236}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 24.533, \Theta^{2266}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 11.685, \Theta^{3311}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 11.685, \Theta^{3314}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 24.533, \Theta^{3344}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 11.685$
85	$\Theta^{1111}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 8.533, \Theta^{1114}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 35.833, \Theta^{1144}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 54.684, \Theta^{1444}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 35.833, \Theta^{2222}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 8.533, \Theta^{2225}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 35.833, \Theta^{2255}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 54.684, \Theta^{2555}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 35.833, \Theta^{3333}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 8.533, \Theta^{3336}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 35.833, \Theta^{3366}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 54.684, \Theta^{3666}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 35.833, \Theta^{4444}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 8.533, \Theta^{5555}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 8.533, \Theta^{6666}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 8.533$
86	$\Theta^{1122}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 8.533, \Theta^{1125}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 17.917, \Theta^{1133}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 8.533, \Theta^{1136}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 17.917, \Theta^{1155}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 8.533, \Theta^{1166}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 8.533, \Theta^{1224}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 17.917, \Theta^{1245}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 37.618, \Theta^{1334}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 17.917, \Theta^{1346}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 37.618, \Theta^{1455}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 17.917, \Theta^{1466}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 17.917, \Theta^{2233}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 8.533, \Theta^{2236}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 17.917, \Theta^{2244}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 8.533, \Theta^{2266}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 8.533, \Theta^{2335}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 17.917, \Theta^{2356}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 37.618, \Theta^{2445}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 17.917, \Theta^{2566}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 17.917, \Theta^{3344}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 8.533, \Theta^{3355}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 8.533, \Theta^{3446}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 17.917, \Theta^{3556}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 17.917, \Theta^{4455}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 8.533, \Theta^{4466}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 8.533, \Theta^{5566}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 8.533$
87	$\Theta^{1113}_{A_{1g}T_{2g}T_{1u}T_{1u}} = 11.685, \Theta^{1116}_{A_{1g}T_{2g}T_{1u}T_{1u}} = 12.267, \Theta^{1134}_{A_{1g}T_{2g}T_{1u}T_{1u}} = 12.267, \Theta^{1146}_{A_{1g}T_{2g}T_{1u}T_{1u}} = 11.685, \Theta^{1212}_{A_{1g}T_{2g}T_{1u}T_{1u}} = 11.685, \Theta^{1215}_{A_{1g}T_{2g}T_{1u}T_{1u}} = 12.267, \Theta^{1224}_{A_{1g}T_{2g}T_{1u}T_{1u}} = 12.267, \Theta^{1245}_{A_{1g}T_{2g}T_{1u}T_{1u}} = 11.685, \Theta^{1323}_{A_{1g}T_{2g}T_{1u}T_{1u}} = -11.685, \Theta^{1326}_{A_{1g}T_{2g}T_{1u}T_{1u}} = -12.267, \Theta^{1335}_{A_{1g}T_{2g}T_{1u}T_{1u}} = -12.267, \Theta^{1356}_{A_{1g}T_{2g}T_{1u}T_{1u}} = -11.685$

88	$\Theta^{1123}_{A_{1g}E_gT_{1u}T_{2u}} = 5.06, \Theta^{1131}_{A_{1g}E_gT_{1u}T_{2u}} = 5.06, \Theta^{1153}_{A_{1g}E_gT_{1u}T_{2u}} = 6.928, \Theta^{1161}_{A_{1g}E_gT_{1u}T_{2u}} = 6.928, \Theta^{1212}_{A_{1g}E_gT_{1u}T_{2u}} = 5.842, \Theta^{1223}_{A_{1g}E_gT_{1u}T_{2u}} = -2.921, \Theta^{1231}_{A_{1g}E_gT_{1u}T_{2u}} = 2.921, \Theta^{1242}_{A_{1g}E_gT_{1u}T_{2u}} = 8.0, \Theta^{1253}_{A_{1g}E_gT_{1u}T_{2u}} = -4.0, \Theta^{1261}_{A_{1g}E_gT_{1u}T_{2u}} = 4.0$
89	$\Theta^{1213}_{T_{1g}T_{1g}T_{2u}T_{2u}} = 16.0, \Theta^{1323}_{T_{1g}T_{1g}T_{2u}T_{2u}} = 16.0, \Theta^{2312}_{T_{1g}T_{1g}T_{2u}T_{2u}} = -16.0$
90	$\Theta^{1123}_{T_{1g}T_{2g}T_{1u}T_{2u}} = -16.0, \Theta^{1153}_{T_{1g}T_{2g}T_{1u}T_{2u}} = -11.685, \Theta^{2231}_{T_{1g}T_{2g}T_{1u}T_{2u}} = 16.0, \Theta^{2261}_{T_{1g}T_{2g}T_{1u}T_{2u}} = 11.685, \Theta^{3312}_{T_{1g}T_{2g}T_{1u}T_{2u}} = -16.0, \Theta^{3342}_{T_{1g}T_{2g}T_{1u}T_{2u}} = -11.685$
91	$\Theta^{1111}_{A_{1g}A_{1g}T_{1g}T_{1g}} = 16.0, \Theta^{1122}_{A_{1g}A_{1g}T_{1g}T_{1g}} = 16.0, \Theta^{1133}_{A_{1g}A_{1g}T_{1g}T_{1g}} = 16.0$
92	$\Theta^{1113}_{E_gT_{1g}T_{1u}T_{1u}} = -3.695, \Theta^{1116}_{E_gT_{1g}T_{1u}T_{1u}} = -5.06, \Theta^{1134}_{E_gT_{1g}T_{1u}T_{1u}} = -5.06, \Theta^{1146}_{E_gT_{1g}T_{1u}T_{1u}} = -6.928, \Theta^{1212}_{E_gT_{1g}T_{1u}T_{1u}} = 3.695, \Theta^{1215}_{E_gT_{1g}T_{1u}T_{1u}} = 5.06, \Theta^{1224}_{E_gT_{1g}T_{1u}T_{1u}} = 5.06, \Theta^{1245}_{E_gT_{1g}T_{1u}T_{1u}} = 6.928, \Theta^{2113}_{E_gT_{1g}T_{1u}T_{1u}} = 2.133, \Theta^{2116}_{E_gT_{1g}T_{1u}T_{1u}} = 2.921, \Theta^{2134}_{E_gT_{1g}T_{1u}T_{1u}} = 2.921, \Theta^{2146}_{E_gT_{1g}T_{1u}T_{1u}} = 4.0, \Theta^{2212}_{E_gT_{1g}T_{1u}T_{1u}} = 2.133, \Theta^{2215}_{E_gT_{1g}T_{1u}T_{1u}} = 2.921, \Theta^{2224}_{E_gT_{1g}T_{1u}T_{1u}} = 2.921, \Theta^{2245}_{E_gT_{1g}T_{1u}T_{1u}} = 4.0, \Theta^{2323}_{E_gT_{1g}T_{1u}T_{1u}} = 4.267, \Theta^{2326}_{E_gT_{1g}T_{1u}T_{1u}} = 5.842, \Theta^{2335}_{E_gT_{1g}T_{1u}T_{1u}} = 5.842, \Theta^{2356}_{E_gT_{1g}T_{1u}T_{1u}} = 8.0$
93	$\Theta^{1111}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 4.267, \Theta^{1114}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 11.685, \Theta^{1133}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -4.267, \Theta^{1136}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -11.685, \Theta^{1144}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 8.0, \Theta^{1166}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -8.0, \Theta^{2211}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -4.267, \Theta^{2214}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -11.685, \Theta^{2222}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 4.267, \Theta^{2225}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 11.685, \Theta^{2244}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -8.0, \Theta^{2255}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 8.0, \Theta^{3322}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -4.267, \Theta^{3325}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -11.685, \Theta^{3333}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 4.267, \Theta^{3336}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 11.685, \Theta^{3355}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -8.0, \Theta^{3366}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 8.0$
94	$\Theta^{1111}_{T_{2g}T_{2g}T_{2u}T_{2u}} = 8.0, \Theta^{1122}_{T_{2g}T_{2g}T_{2u}T_{2u}} = 8.0, \Theta^{2222}_{T_{2g}T_{2g}T_{2u}T_{2u}} = 8.0, \Theta^{2233}_{T_{2g}T_{2g}T_{2u}T_{2u}} = 8.0, \Theta^{3311}_{T_{2g}T_{2g}T_{2u}T_{2u}} = 8.0, \Theta^{3333}_{T_{2g}T_{2g}T_{2u}T_{2u}} = 8.0$
95	$\Theta^{1212}_{T_{1g}T_{1g}T_{2g}T_{2g}} = 16.0, \Theta^{1313}_{T_{1g}T_{1g}T_{2g}T_{2g}} = 16.0, \Theta^{2323}_{T_{1g}T_{1g}T_{2g}T_{2g}} = 16.0$
96	$\Theta^{1122}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 16.0, \Theta^{1422}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 23.369, \Theta^{2233}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 16.0, \Theta^{2533}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 23.369, \Theta^{3311}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 16.0, \Theta^{3611}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 23.369, \Theta^{4422}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 8.533, \Theta^{5533}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 8.533, \Theta^{6611}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 8.533$
97	$\Theta^{1123}_{E_gT_{1g}T_{2g}T_{2g}} = 13.856, \Theta^{1213}_{E_gT_{1g}T_{2g}T_{2g}} = -13.856, \Theta^{2123}_{E_gT_{1g}T_{2g}T_{2g}} = -8.0, \Theta^{2213}_{E_gT_{1g}T_{2g}T_{2g}} = -8.0, \Theta^{2312}_{E_gT_{1g}T_{2g}T_{2g}} = 16.0$
98	$\Theta^{1221}_{T_{2g}T_{2g}T_{1u}T_{2u}} = 5.842, \Theta^{1233}_{T_{2g}T_{2g}T_{1u}T_{2u}} = 5.842, \Theta^{1251}_{T_{2g}T_{2g}T_{1u}T_{2u}} = 8.0, \Theta^{1263}_{T_{2g}T_{2g}T_{1u}T_{2u}} = 8.0, \Theta^{1313}_{T_{2g}T_{2g}T_{1u}T_{2u}} = 5.842, \Theta^{1322}_{T_{2g}T_{2g}T_{1u}T_{2u}} = -5.842, \Theta^{1343}_{T_{2g}T_{2g}T_{1u}T_{2u}} = 8.0, \Theta^{1352}_{T_{2g}T_{2g}T_{1u}T_{2u}} = -8.0, \Theta^{2311}_{T_{2g}T_{2g}T_{1u}T_{2u}} = 5.842, \Theta^{2332}_{T_{2g}T_{2g}T_{1u}T_{2u}} = 5.842, \Theta^{2341}_{T_{2g}T_{2g}T_{1u}T_{2u}} = 8.0, \Theta^{2362}_{T_{2g}T_{2g}T_{1u}T_{2u}} = 8.0$

99	$\Theta^{1122}_{T_{1g}T_{1g}T_{2g}} = 8.0, \Theta^{1133}_{T_{1g}T_{1g}T_{2g}} = -8.0, \Theta^{1221}_{T_{1g}T_{1g}T_{2g}} = -8.0, \Theta^{1331}_{T_{1g}T_{1g}T_{2g}} = 8.0, \Theta^{2233}_{T_{1g}T_{1g}T_{2g}} = 8.0, \Theta^{2332}_{T_{1g}T_{1g}T_{2g}} = -8.0$
100	$\Theta^{1111}_{A_{1g}E_gT_{1u}T_{1u}} = 13.856, \Theta^{1114}_{A_{1g}E_gT_{1u}T_{1u}} = 20.239, \Theta^{1122}_{A_{1g}E_gT_{1u}T_{1u}} = -6.928, \Theta^{1125}_{A_{1g}E_gT_{1u}T_{1u}} = -10.119, \Theta^{1133}_{A_{1g}E_gT_{1u}T_{1u}} = -6.928, \Theta^{1136}_{A_{1g}E_gT_{1u}T_{1u}} = -10.119, \Theta^{1144}_{A_{1g}E_gT_{1u}T_{1u}} = 7.39, \Theta^{1155}_{A_{1g}E_gT_{1u}T_{1u}} = -3.695, \Theta^{1166}_{A_{1g}E_gT_{1u}T_{1u}} = -3.695, \Theta^{1222}_{A_{1g}E_gT_{1u}T_{1u}} = -12.0, \Theta^{1225}_{A_{1g}E_gT_{1u}T_{1u}} = -17.527, \Theta^{1233}_{A_{1g}E_gT_{1u}T_{1u}} = 12.0, \Theta^{1236}_{A_{1g}E_gT_{1u}T_{1u}} = 17.527, \Theta^{1255}_{A_{1g}E_gT_{1u}T_{1u}} = -6.4, \Theta^{1266}_{A_{1g}E_gT_{1u}T_{1u}} = 6.4$
101	$\Theta^{1111}_{A_{1g}A_{1g}T_{1u}T_{1u}} = 11.685, \Theta^{1114}_{A_{1g}A_{1g}T_{1u}T_{1u}} = 24.533, \Theta^{1122}_{A_{1g}A_{1g}T_{1u}T_{1u}} = 11.685, \Theta^{1125}_{A_{1g}A_{1g}T_{1u}T_{1u}} = 24.533, \Theta^{1133}_{A_{1g}A_{1g}T_{1u}T_{1u}} = 11.685, \Theta^{1136}_{A_{1g}A_{1g}T_{1u}T_{1u}} = 24.533, \Theta^{1144}_{A_{1g}A_{1g}T_{1u}T_{1u}} = 11.685, \Theta^{1155}_{A_{1g}A_{1g}T_{1u}T_{1u}} = 11.685, \Theta^{1166}_{A_{1g}A_{1g}T_{1u}T_{1u}} = 11.685$
102	$\Theta^{1111}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 8.0, \Theta^{1114}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 11.685, \Theta^{1133}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 8.0, \Theta^{1136}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 11.685, \Theta^{1144}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 4.267, \Theta^{1166}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 4.267, \Theta^{2211}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 8.0, \Theta^{2214}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 11.685, \Theta^{2222}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 8.0, \Theta^{2225}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 11.685, \Theta^{2244}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 4.267, \Theta^{2255}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 4.267, \Theta^{3322}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 8.0, \Theta^{3325}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 11.685, \Theta^{3333}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 8.0, \Theta^{3336}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 11.685, \Theta^{3355}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 4.267, \Theta^{3366}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 4.267$
103	$\Theta^{1122}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 6.232, \Theta^{1125}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 15.076, \Theta^{1133}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 6.232, \Theta^{1136}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 15.076, \Theta^{1155}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 8.958, \Theta^{1166}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 8.958, \Theta^{1224}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 15.076, \Theta^{1245}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 35.833, \Theta^{1334}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 15.076, \Theta^{1346}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 35.833, \Theta^{1455}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 20.8, \Theta^{1466}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 20.8, \Theta^{2233}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 6.232, \Theta^{2236}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 15.076, \Theta^{2244}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 8.958, \Theta^{2266}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 8.958, \Theta^{2335}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 15.076, \Theta^{2356}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 35.833, \Theta^{2445}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 20.8, \Theta^{2566}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 20.8, \Theta^{3344}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 8.958, \Theta^{3355}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 8.958, \Theta^{3446}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 20.8, \Theta^{3556}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 20.8, \Theta^{4455}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 11.685, \Theta^{4466}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 11.685, \Theta^{5566}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 11.685$
104	$\Theta^{1223}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -8.0, \Theta^{1226}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -5.842, \Theta^{1235}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -5.842, \Theta^{1256}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -4.267, \Theta^{1312}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -8.0, \Theta^{1315}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -5.842, \Theta^{1324}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -5.842, \Theta^{1345}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -4.267, \Theta^{2123}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 8.0, \Theta^{2126}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 5.842, \Theta^{2135}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 5.842, \Theta^{2156}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 4.267, \Theta^{2313}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 8.0, \Theta^{2316}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 5.842, \Theta^{2334}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 5.842, \Theta^{2346}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 4.267, \Theta^{3112}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 8.0, \Theta^{3115}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 5.842, \Theta^{3124}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 5.842, \Theta^{3145}_{T_{1g}T_{2g}T_{1u}T_{1u}} = 4.267, \Theta^{3213}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -8.0, \Theta^{3216}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -5.842, \Theta^{3234}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -5.842, \Theta^{3246}_{T_{1g}T_{2g}T_{1u}T_{1u}} = -4.267$

105	$\Theta^{1221}_{T_{2g}T_{2g}T_{1u}T_{2u}} = 8.0, \Theta^{1233}_{T_{2g}T_{2g}T_{1u}T_{2u}} = 8.0, \Theta^{1251}_{T_{2g}T_{2g}T_{1u}T_{2u}} = 5.842, \Theta^{1263}_{T_{2g}T_{2g}T_{1u}T_{2u}} = 5.842, \Theta^{1313}_{T_{2g}T_{2g}T_{1u}T_{2u}} = 8.0, \Theta^{1322}_{T_{2g}T_{2g}T_{1u}T_{2u}} = -8.0, \Theta^{1343}_{T_{2g}T_{2g}T_{1u}T_{2u}} = 5.842, \Theta^{1352}_{T_{2g}T_{2g}T_{1u}T_{2u}} = -5.842, \Theta^{2311}_{T_{2g}T_{2g}T_{1u}T_{2u}} = 8.0, \Theta^{2332}_{T_{2g}T_{2g}T_{1u}T_{2u}} = 8.0, \Theta^{2341}_{T_{2g}T_{2g}T_{1u}T_{2u}} = 5.842, \Theta^{2362}_{T_{2g}T_{2g}T_{1u}T_{2u}} = 5.842$
106	$\Theta^{1223}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 11.685, \Theta^{1312}_{T_{1u}T_{1u}T_{2u}T_{2u}} = -11.685, \Theta^{1523}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 12.267, \Theta^{1612}_{T_{1u}T_{1u}T_{2u}T_{2u}} = -12.267, \Theta^{2313}_{T_{1u}T_{1u}T_{2u}T_{2u}} = -11.685, \Theta^{2423}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 12.267, \Theta^{2613}_{T_{1u}T_{1u}T_{2u}T_{2u}} = -12.267, \Theta^{3412}_{T_{1u}T_{1u}T_{2u}T_{2u}} = -12.267, \Theta^{3513}_{T_{1u}T_{1u}T_{2u}T_{2u}} = -12.267, \Theta^{4523}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 11.685, \Theta^{4612}_{T_{1u}T_{1u}T_{2u}T_{2u}} = -11.685, \Theta^{5613}_{T_{1u}T_{1u}T_{2u}T_{2u}} = -11.685$
107	$\Theta^{1111}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 4.267, \Theta^{1114}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 11.685, \Theta^{1133}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 4.267, \Theta^{1136}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 11.685, \Theta^{1144}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 8.0, \Theta^{1166}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 8.0, \Theta^{2211}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 4.267, \Theta^{2214}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 11.685, \Theta^{2222}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 4.267, \Theta^{2225}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 11.685, \Theta^{2244}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 8.0, \Theta^{2255}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 8.0, \Theta^{3322}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 4.267, \Theta^{3325}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 11.685, \Theta^{3333}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 4.267, \Theta^{3336}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 11.685, \Theta^{3355}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 8.0, \Theta^{3366}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 8.0$
108	$\Theta^{1111}_{A_{1g}T_{2g}T_{1u}T_{2u}} = -8.0, \Theta^{1132}_{A_{1g}T_{2g}T_{1u}T_{2u}} = -8.0, \Theta^{1141}_{A_{1g}T_{2g}T_{1u}T_{2u}} = -5.842, \Theta^{1162}_{A_{1g}T_{2g}T_{1u}T_{2u}} = -5.842, \Theta^{1213}_{A_{1g}T_{2g}T_{1u}T_{2u}} = -8.0, \Theta^{1222}_{A_{1g}T_{2g}T_{1u}T_{2u}} = 8.0, \Theta^{1243}_{A_{1g}T_{2g}T_{1u}T_{2u}} = -5.842, \Theta^{1252}_{A_{1g}T_{2g}T_{1u}T_{2u}} = 5.842, \Theta^{1321}_{A_{1g}T_{2g}T_{1u}T_{2u}} = -8.0, \Theta^{1333}_{A_{1g}T_{2g}T_{1u}T_{2u}} = -8.0, \Theta^{1351}_{A_{1g}T_{2g}T_{1u}T_{2u}} = -5.842, \Theta^{1363}_{A_{1g}T_{2g}T_{1u}T_{2u}} = -5.842$
109	$\Theta^{1223}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 8.533, \Theta^{1226}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 11.685, \Theta^{1235}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 11.685, \Theta^{1256}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 16.0, \Theta^{1312}_{T_{2g}T_{2g}T_{1u}T_{1u}} = -8.533, \Theta^{1315}_{T_{2g}T_{2g}T_{1u}T_{1u}} = -11.685, \Theta^{1324}_{T_{2g}T_{2g}T_{1u}T_{1u}} = -11.685, \Theta^{1345}_{T_{2g}T_{2g}T_{1u}T_{1u}} = -16.0, \Theta^{2313}_{T_{2g}T_{2g}T_{1u}T_{1u}} = -8.533, \Theta^{2316}_{T_{2g}T_{2g}T_{1u}T_{1u}} = -11.685, \Theta^{2334}_{T_{2g}T_{2g}T_{1u}T_{1u}} = -11.685, \Theta^{2346}_{T_{2g}T_{2g}T_{1u}T_{1u}} = -16.0$
110	$\Theta^{1111}_{T_{2g}T_{2g}T_{2g}T_{2g}} = 16.0, \Theta^{2222}_{T_{2g}T_{2g}T_{2g}T_{2g}} = 16.0, \Theta^{3333}_{T_{2g}T_{2g}T_{2g}T_{2g}} = 16.0$
111	$\Theta^{1111}_{T_{1g}T_{1g}T_{1g}T_{1g}} = 16.0, \Theta^{2222}_{T_{1g}T_{1g}T_{1g}T_{1g}} = 16.0, \Theta^{3333}_{T_{1g}T_{1g}T_{1g}T_{1g}} = 16.0$
112	$\Theta^{1111}_{E_gE_gT_{2u}T_{2u}} = 6.0, \Theta^{1122}_{E_gE_gT_{2u}T_{2u}} = 12.0, \Theta^{1133}_{E_gE_gT_{2u}T_{2u}} = 6.0, \Theta^{1211}_{E_gE_gT_{2u}T_{2u}} = -6.928, \Theta^{1233}_{E_gE_gT_{2u}T_{2u}} = 6.928, \Theta^{2211}_{E_gE_gT_{2u}T_{2u}} = 10.0, \Theta^{2222}_{E_gE_gT_{2u}T_{2u}} = 4.0, \Theta^{2233}_{E_gE_gT_{2u}T_{2u}} = 10.0$
113	$\Theta^{1111}_{E_gE_gT_{1g}T_{1g}} = 6.0, \Theta^{1122}_{E_gE_gT_{1g}T_{1g}} = 6.0, \Theta^{1133}_{E_gE_gT_{1g}T_{1g}} = 12.0, \Theta^{1211}_{E_gE_gT_{1g}T_{1g}} = 6.928, \Theta^{1222}_{E_gE_gT_{1g}T_{1g}} = -6.928, \Theta^{2211}_{E_gE_gT_{1g}T_{1g}} = 10.0, \Theta^{2222}_{E_gE_gT_{1g}T_{1g}} = 10.0, \Theta^{2233}_{E_gE_gT_{1g}T_{1g}} = 4.0$
114	$\Theta^{1122}_{T_{2u}T_{2u}T_{2u}T_{2u}} = 16.0, \Theta^{1133}_{T_{2u}T_{2u}T_{2u}T_{2u}} = 16.0, \Theta^{2233}_{T_{2u}T_{2u}T_{2u}T_{2u}} = 16.0$

115	$\Theta^{1111}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 6.232, \Theta^{1114}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 30.151, \Theta^{1144}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 53.75, \Theta^{1444}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 41.6, \Theta^{2222}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 6.232, \Theta^{2225}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 30.151, \Theta^{2255}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 53.75, \Theta^{2555}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 41.6, \Theta^{3333}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 6.232, \Theta^{3336}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 30.151, \Theta^{3366}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 53.75, \Theta^{3666}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 41.6, \Theta^{4444}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 11.685, \Theta^{5555}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 11.685, \Theta^{6666}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 11.685$
116	$\Theta^{1111}_{T_{1g}T_{2g}T_{2u}T_{2u}} = -8.0, \Theta^{1122}_{T_{1g}T_{2g}T_{2u}T_{2u}} = 8.0, \Theta^{2222}_{T_{1g}T_{2g}T_{2u}T_{2u}} = -8.0, \Theta^{2233}_{T_{1g}T_{2g}T_{2u}T_{2u}} = 8.0, \Theta^{3311}_{T_{1g}T_{2g}T_{2u}T_{2u}} = 8.0, \Theta^{3333}_{T_{1g}T_{2g}T_{2u}T_{2u}} = -8.0$
117	$\Theta^{1111}_{E_gE_gT_{1u}T_{1u}} = 2.921, \Theta^{1114}_{E_gE_gT_{1u}T_{1u}} = 6.133, \Theta^{1122}_{E_gE_gT_{1u}T_{1u}} = 7.303, \Theta^{1125}_{E_gE_gT_{1u}T_{1u}} = 15.333, \Theta^{1133}_{E_gE_gT_{1u}T_{1u}} = 7.303, \Theta^{1136}_{E_gE_gT_{1u}T_{1u}} = 15.333, \Theta^{1144}_{E_gE_gT_{1u}T_{1u}} = 2.921, \Theta^{1155}_{E_gE_gT_{1u}T_{1u}} = 7.303, \Theta^{1166}_{E_gE_gT_{1u}T_{1u}} = 7.303, \Theta^{1222}_{E_gE_gT_{1u}T_{1u}} = -5.06, \Theta^{1225}_{E_gE_gT_{1u}T_{1u}} = -10.623, \Theta^{1233}_{E_gE_gT_{1u}T_{1u}} = 5.06, \Theta^{1236}_{E_gE_gT_{1u}T_{1u}} = 10.623, \Theta^{1255}_{E_gE_gT_{1u}T_{1u}} = -5.06, \Theta^{1266}_{E_gE_gT_{1u}T_{1u}} = 5.06, \Theta^{2211}_{E_gE_gT_{1u}T_{1u}} = 8.764, \Theta^{2214}_{E_gE_gT_{1u}T_{1u}} = 18.4, \Theta^{2222}_{E_gE_gT_{1u}T_{1u}} = 4.382, \Theta^{2225}_{E_gE_gT_{1u}T_{1u}} = 9.2, \Theta^{2233}_{E_gE_gT_{1u}T_{1u}} = 4.382, \Theta^{2236}_{E_gE_gT_{1u}T_{1u}} = 9.2, \Theta^{2244}_{E_gE_gT_{1u}T_{1u}} = 8.764, \Theta^{2255}_{E_gE_gT_{1u}T_{1u}} = 4.382, \Theta^{2266}_{E_gE_gT_{1u}T_{1u}} = 4.382$
118	$\Theta^{1111}_{E_gT_{1g}T_{1u}T_{2u}} = 4.0, \Theta^{1132}_{E_gT_{1g}T_{1u}T_{2u}} = 8.0, \Theta^{1141}_{E_gT_{1g}T_{1u}T_{2u}} = 2.921, \Theta^{1162}_{E_gT_{1g}T_{1u}T_{2u}} = 5.842, \Theta^{1213}_{E_gT_{1g}T_{1u}T_{2u}} = -4.0, \Theta^{1222}_{E_gT_{1g}T_{1u}T_{2u}} = 8.0, \Theta^{1243}_{E_gT_{1g}T_{1u}T_{2u}} = -2.921, \Theta^{1252}_{E_gT_{1g}T_{1u}T_{2u}} = 5.842, \Theta^{1321}_{E_gT_{1g}T_{1u}T_{2u}} = -4.0, \Theta^{1333}_{E_gT_{1g}T_{1u}T_{2u}} = 4.0, \Theta^{1351}_{E_gT_{1g}T_{1u}T_{2u}} = -2.921, \Theta^{1363}_{E_gT_{1g}T_{1u}T_{2u}} = 2.921, \Theta^{2111}_{E_gT_{1g}T_{1u}T_{2u}} = -6.928, \Theta^{2141}_{E_gT_{1g}T_{1u}T_{2u}} = -5.06, \Theta^{2213}_{E_gT_{1g}T_{1u}T_{2u}} = -6.928, \Theta^{2243}_{E_gT_{1g}T_{1u}T_{2u}} = -5.06, \Theta^{2321}_{E_gT_{1g}T_{1u}T_{2u}} = 6.928, \Theta^{2333}_{E_gT_{1g}T_{1u}T_{2u}} = 6.928, \Theta^{2351}_{E_gT_{1g}T_{1u}T_{2u}} = 5.06, \Theta^{2363}_{E_gT_{1g}T_{1u}T_{2u}} = 5.06$
119	$\Theta^{1122}_{T_{2g}T_{2g}T_{2g}T_{2g}} = 16.0, \Theta^{1133}_{T_{2g}T_{2g}T_{2g}T_{2g}} = 16.0, \Theta^{2233}_{T_{2g}T_{2g}T_{2g}T_{2g}} = 16.0$
120	$\Theta^{1233}_{T_{1g}T_{2g}T_{1u}T_{2u}} = -8.0, \Theta^{1263}_{T_{1g}T_{2g}T_{1u}T_{2u}} = -5.842, \Theta^{1313}_{T_{1g}T_{2g}T_{1u}T_{2u}} = 8.0, \Theta^{1343}_{T_{1g}T_{2g}T_{1u}T_{2u}} = 5.842, \Theta^{2121}_{T_{1g}T_{2g}T_{1u}T_{2u}} = 8.0, \Theta^{2151}_{T_{1g}T_{2g}T_{1u}T_{2u}} = 5.842, \Theta^{2311}_{T_{1g}T_{2g}T_{1u}T_{2u}} = -8.0, \Theta^{2341}_{T_{1g}T_{2g}T_{1u}T_{2u}} = -5.842, \Theta^{3122}_{T_{1g}T_{2g}T_{1u}T_{2u}} = 8.0, \Theta^{3152}_{T_{1g}T_{2g}T_{1u}T_{2u}} = 5.842, \Theta^{3232}_{T_{1g}T_{2g}T_{1u}T_{2u}} = 8.0, \Theta^{3262}_{T_{1g}T_{2g}T_{1u}T_{2u}} = 5.842$
121	$\Theta^{1223}_{T_{1u}T_{1u}T_{2u}T_{2u}} = -16.0, \Theta^{1312}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 16.0, \Theta^{1523}_{T_{1u}T_{1u}T_{2u}T_{2u}} = -11.685, \Theta^{1612}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 11.685, \Theta^{2313}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 16.0, \Theta^{2423}_{T_{1u}T_{1u}T_{2u}T_{2u}} = -11.685, \Theta^{2613}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 11.685, \Theta^{3412}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 11.685, \Theta^{3513}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 11.685, \Theta^{4523}_{T_{1u}T_{1u}T_{2u}T_{2u}} = -8.533, \Theta^{4612}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 8.533, \Theta^{5613}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 8.533$

122	$\Theta^{1111}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 8.0, \Theta^{1114}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 11.685, \Theta^{1133}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 8.0, \Theta^{1136}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 11.685, \Theta^{1144}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 4.267, \Theta^{1166}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 4.267, \Theta^{2211}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 8.0, \Theta^{2214}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 11.685, \Theta^{2222}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 8.0, \Theta^{2225}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 11.685, \Theta^{2244}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 4.267, \Theta^{2255}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 4.267, \Theta^{3322}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 8.0, \Theta^{3325}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 11.685, \Theta^{3333}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 8.0, \Theta^{3336}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 11.685, \Theta^{3355}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 4.267, \Theta^{3366}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 4.267$
123	$\Theta^{1122}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 16.0, \Theta^{1125}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 23.369, \Theta^{1133}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 16.0, \Theta^{1136}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 23.369, \Theta^{1155}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 8.533, \Theta^{1166}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 8.533, \Theta^{1224}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 23.369, \Theta^{1245}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 34.133, \Theta^{1334}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 23.369, \Theta^{1346}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 34.133, \Theta^{1455}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 12.464, \Theta^{1466}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 12.464, \Theta^{2233}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 16.0, \Theta^{2236}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 23.369, \Theta^{2244}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 8.533, \Theta^{2266}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 8.533, \Theta^{2335}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 23.369, \Theta^{2356}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 34.133, \Theta^{2445}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 12.464, \Theta^{2566}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 12.464, \Theta^{3344}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 8.533, \Theta^{3355}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 8.533, \Theta^{3446}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 12.464, \Theta^{3556}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 12.464, \Theta^{4455}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 4.551, \Theta^{4466}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 4.551, \Theta^{5566}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 4.551$
124	$\Theta^{1122}_{T_{1g}T_{1g}T_{1g}T_{1g}} = 16.0, \Theta^{1133}_{T_{1g}T_{1g}T_{1g}T_{1g}} = 16.0, \Theta^{2233}_{T_{1g}T_{1g}T_{1g}T_{1g}} = 16.0$
125	$\Theta^{1111}_{E_gE_gT_{2g}T_{2g}} = 3.464, \Theta^{1122}_{E_gE_gT_{2g}T_{2g}} = 3.464, \Theta^{1133}_{E_gE_gT_{2g}T_{2g}} = -6.928, \Theta^{1211}_{E_gE_gT_{2g}T_{2g}} = -12.0, \Theta^{1222}_{E_gE_gT_{2g}T_{2g}} = 12.0, \Theta^{2211}_{E_gE_gT_{2g}T_{2g}} = -3.464, \Theta^{2222}_{E_gE_gT_{2g}T_{2g}} = -3.464, \Theta^{2233}_{E_gE_gT_{2g}T_{2g}} = 6.928$
126	$\Theta^{1111}_{A_{1g}E_gT_{1g}T_{1g}} = -6.928, \Theta^{1122}_{A_{1g}E_gT_{1g}T_{1g}} = -6.928, \Theta^{1133}_{A_{1g}E_gT_{1g}T_{1g}} = 13.856, \Theta^{1211}_{A_{1g}E_gT_{1g}T_{1g}} = -12.0, \Theta^{1222}_{A_{1g}E_gT_{1g}T_{1g}} = 12.0$
127	$\Theta^{1223}_{T_{1g}T_{1g}T_{1u}T_{1u}} = -16.0, \Theta^{1226}_{T_{1g}T_{1g}T_{1u}T_{1u}} = -11.685, \Theta^{1235}_{T_{1g}T_{1g}T_{1u}T_{1u}} = -11.685, \Theta^{1256}_{T_{1g}T_{1g}T_{1u}T_{1u}} = -8.533, \Theta^{1312}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 16.0, \Theta^{1315}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 11.685, \Theta^{1324}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 11.685, \Theta^{1345}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 8.533, \Theta^{2313}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 16.0, \Theta^{2316}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 11.685, \Theta^{2334}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 11.685, \Theta^{2346}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 8.533$
128	$\Theta^{1122}_{T_{1g}T_{2g}T_{2g}T_{2g}} = -8.0, \Theta^{1133}_{T_{1g}T_{2g}T_{2g}T_{2g}} = 8.0, \Theta^{2112}_{T_{1g}T_{2g}T_{2g}T_{2g}} = 8.0, \Theta^{2233}_{T_{1g}T_{2g}T_{2g}T_{2g}} = -8.0, \Theta^{3113}_{T_{1g}T_{2g}T_{2g}T_{2g}} = -8.0, \Theta^{3223}_{T_{1g}T_{2g}T_{2g}T_{2g}} = 8.0$
129	$\Theta^{1113}_{E_gT_{2g}T_{1u}T_{1u}} = -6.928, \Theta^{1116}_{E_gT_{2g}T_{1u}T_{1u}} = -5.06, \Theta^{1134}_{E_gT_{2g}T_{1u}T_{1u}} = -5.06, \Theta^{1146}_{E_gT_{2g}T_{1u}T_{1u}} = -3.695, \Theta^{1212}_{E_gT_{2g}T_{1u}T_{1u}} = -6.928, \Theta^{1215}_{E_gT_{2g}T_{1u}T_{1u}} = -5.06, \Theta^{1224}_{E_gT_{2g}T_{1u}T_{1u}} = -5.06, \Theta^{1245}_{E_gT_{2g}T_{1u}T_{1u}} = -3.695, \Theta^{1323}_{E_gT_{2g}T_{1u}T_{1u}} = -13.856, \Theta^{1326}_{E_gT_{2g}T_{1u}T_{1u}} = -10.119, \Theta^{1335}_{E_gT_{2g}T_{1u}T_{1u}} = -10.119, \Theta^{1356}_{E_gT_{2g}T_{1u}T_{1u}} = -7.39, \Theta^{2113}_{E_gT_{2g}T_{1u}T_{1u}} = -12.0, \Theta^{2116}_{E_gT_{2g}T_{1u}T_{1u}} = -8.764, \Theta^{2134}_{E_gT_{2g}T_{1u}T_{1u}} = -8.764, \Theta^{2146}_{E_gT_{2g}T_{1u}T_{1u}} = -6.4, \Theta^{2212}_{E_gT_{2g}T_{1u}T_{1u}} = 12.0, \Theta^{2215}_{E_gT_{2g}T_{1u}T_{1u}} = 8.764, \Theta^{2224}_{E_gT_{2g}T_{1u}T_{1u}} = 8.764, \Theta^{2245}_{E_gT_{2g}T_{1u}T_{1u}} = 6.4$

130	$\Theta^{1111}_{A_{1g}A_{1g}T_{1u}T_{1u}} = 8.533, \Theta^{1114}_{A_{1g}A_{1g}T_{1u}T_{1u}} = 23.369, \Theta^{1122}_{A_{1g}A_{1g}T_{1u}T_{1u}} = 8.533, \Theta^{1125}_{A_{1g}A_{1g}T_{1u}T_{1u}} = 23.369, \Theta^{1133}_{A_{1g}A_{1g}T_{1u}T_{1u}} = 8.533, \Theta^{1136}_{A_{1g}A_{1g}T_{1u}T_{1u}} = 23.369, \Theta^{1144}_{A_{1g}A_{1g}T_{1u}T_{1u}} = 16.0, \Theta^{1155}_{A_{1g}A_{1g}T_{1u}T_{1u}} = 16.0, \Theta^{1166}_{A_{1g}A_{1g}T_{1u}T_{1u}} = 16.0$
131	$\Theta^{1122}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 8.533, \Theta^{1422}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 23.369, \Theta^{2233}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 8.533, \Theta^{2533}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 23.369, \Theta^{3311}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 8.533, \Theta^{3611}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 23.369, \Theta^{4422}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 16.0, \Theta^{5533}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 16.0, \Theta^{6611}_{T_{1u}T_{1u}T_{2u}T_{2u}} = 16.0$
132	$\Theta^{1111}_{A_{1g}A_{1g}T_{2u}T_{2u}} = 16.0, \Theta^{1122}_{A_{1g}A_{1g}T_{2u}T_{2u}} = 16.0, \Theta^{1133}_{A_{1g}A_{1g}T_{2u}T_{2u}} = 16.0$
133	$\Theta^{1123}_{A_{1g}E_gT_{1u}T_{2u}} = 13.856, \Theta^{1131}_{A_{1g}E_gT_{1u}T_{2u}} = 13.856, \Theta^{1153}_{A_{1g}E_gT_{1u}T_{2u}} = 10.119, \Theta^{1161}_{A_{1g}E_gT_{1u}T_{2u}} = 10.119, \Theta^{1212}_{A_{1g}E_gT_{1u}T_{2u}} = 16.0, \Theta^{1223}_{A_{1g}E_gT_{1u}T_{2u}} = -8.0, \Theta^{1231}_{A_{1g}E_gT_{1u}T_{2u}} = 8.0, \Theta^{1242}_{A_{1g}E_gT_{1u}T_{2u}} = 11.685, \Theta^{1253}_{A_{1g}E_gT_{1u}T_{2u}} = -5.842, \Theta^{1261}_{A_{1g}E_gT_{1u}T_{2u}} = 5.842$
134	$\Theta^{1111}_{E_gE_gT_{2g}T_{2g}} = 6.0, \Theta^{1122}_{E_gE_gT_{2g}T_{2g}} = 6.0, \Theta^{1133}_{E_gE_gT_{2g}T_{2g}} = 12.0, \Theta^{1211}_{E_gE_gT_{2g}T_{2g}} = 6.928, \Theta^{1222}_{E_gE_gT_{2g}T_{2g}} = -6.928, \Theta^{2211}_{E_gE_gT_{2g}T_{2g}} = 10.0, \Theta^{2222}_{E_gE_gT_{2g}T_{2g}} = 10.0, \Theta^{2233}_{E_gE_gT_{2g}T_{2g}} = 4.0$
135	$\Theta^{1111}_{E_gE_gE_gE_g} = 6.0, \Theta^{1122}_{E_gE_gE_gE_g} = 12.0, \Theta^{2222}_{E_gE_gE_gE_g} = 6.0$
136	$\Theta^{1111}_{A_{1g}A_{1g}A_{1g}A_{1g}} = 48.0$
137	$\Theta^{1113}_{E_gT_{2g}T_{1u}T_{1u}} = 4.267, \Theta^{1116}_{E_gT_{2g}T_{1u}T_{1u}} = 5.842, \Theta^{1134}_{E_gT_{2g}T_{1u}T_{1u}} = 5.842, \Theta^{1146}_{E_gT_{2g}T_{1u}T_{1u}} = 8.0, \Theta^{1212}_{E_gT_{2g}T_{1u}T_{1u}} = 4.267, \Theta^{1215}_{E_gT_{2g}T_{1u}T_{1u}} = 5.842, \Theta^{1224}_{E_gT_{2g}T_{1u}T_{1u}} = 5.842, \Theta^{1245}_{E_gT_{2g}T_{1u}T_{1u}} = 8.0, \Theta^{1323}_{E_gT_{2g}T_{1u}T_{1u}} = 8.533, \Theta^{1326}_{E_gT_{2g}T_{1u}T_{1u}} = 11.685, \Theta^{1335}_{E_gT_{2g}T_{1u}T_{1u}} = 11.685, \Theta^{1356}_{E_gT_{2g}T_{1u}T_{1u}} = 16.0, \Theta^{2113}_{E_gT_{2g}T_{1u}T_{1u}} = 7.39, \Theta^{2116}_{E_gT_{2g}T_{1u}T_{1u}} = 10.119, \Theta^{2134}_{E_gT_{2g}T_{1u}T_{1u}} = 10.119, \Theta^{2146}_{E_gT_{2g}T_{1u}T_{1u}} = 13.856, \Theta^{2212}_{E_gT_{2g}T_{1u}T_{1u}} = -7.39, \Theta^{2215}_{E_gT_{2g}T_{1u}T_{1u}} = -10.119, \Theta^{2224}_{E_gT_{2g}T_{1u}T_{1u}} = -10.119, \Theta^{2245}_{E_gT_{2g}T_{1u}T_{1u}} = -13.856$
138	$\Theta^{1122}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 16.0, \Theta^{1125}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 23.369, \Theta^{1155}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 8.533, \Theta^{2233}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 16.0, \Theta^{2236}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 23.369, \Theta^{2266}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 8.533, \Theta^{3311}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 16.0, \Theta^{3314}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 23.369, \Theta^{3344}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 8.533$
139	$\Theta^{1111}_{A_{1g}T_{1g}T_{1u}T_{2u}} = -8.0, \Theta^{1132}_{A_{1g}T_{1g}T_{1u}T_{2u}} = 8.0, \Theta^{1141}_{A_{1g}T_{1g}T_{1u}T_{2u}} = -5.842, \Theta^{1162}_{A_{1g}T_{1g}T_{1u}T_{2u}} = 5.842, \Theta^{1213}_{A_{1g}T_{1g}T_{1u}T_{2u}} = 8.0, \Theta^{1222}_{A_{1g}T_{1g}T_{1u}T_{2u}} = 8.0, \Theta^{1243}_{A_{1g}T_{1g}T_{1u}T_{2u}} = 5.842, \Theta^{1252}_{A_{1g}T_{1g}T_{1u}T_{2u}} = 5.842, \Theta^{1321}_{A_{1g}T_{1g}T_{1u}T_{2u}} = 8.0, \Theta^{1333}_{A_{1g}T_{1g}T_{1u}T_{2u}} = -8.0, \Theta^{1351}_{A_{1g}T_{1g}T_{1u}T_{2u}} = 5.842, \Theta^{1363}_{A_{1g}T_{1g}T_{1u}T_{2u}} = -5.842$

140	$\Theta^{1111}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 5.842, \Theta^{1114}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 12.267, \Theta^{1133}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 5.842, \Theta^{1136}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 12.267, \Theta^{1144}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 5.842, \Theta^{1166}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 5.842, \Theta^{2211}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 5.842, \Theta^{2214}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 12.267, \Theta^{2222}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 5.842, \Theta^{2225}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 12.267, \Theta^{2244}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 5.842, \Theta^{2255}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 5.842, \Theta^{3322}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 5.842, \Theta^{3325}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 12.267, \Theta^{3333}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 5.842, \Theta^{3336}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 12.267, \Theta^{3355}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 5.842, \Theta^{3366}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 5.842$
141	$\Theta^{1111}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 4.551, \Theta^{1114}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 24.927, \Theta^{1144}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 51.2, \Theta^{1444}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 46.739, \Theta^{2222}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 4.551, \Theta^{2225}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 24.927, \Theta^{2255}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 51.2, \Theta^{2555}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 46.739, \Theta^{3333}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 4.551, \Theta^{3336}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 24.927, \Theta^{3366}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 51.2, \Theta^{3666}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 46.739, \Theta^{4444}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 16.0, \Theta^{5555}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 16.0, \Theta^{6666}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 16.0$
142	$\Theta^{1111}_{E_gE_gT_{1u}T_{1u}} = 4.0, \Theta^{1114}_{E_gE_gT_{1u}T_{1u}} = 5.842, \Theta^{1122}_{E_gE_gT_{1u}T_{1u}} = 10.0, \Theta^{1125}_{E_gE_gT_{1u}T_{1u}} = 14.606, \Theta^{1133}_{E_gE_gT_{1u}T_{1u}} = 10.0, \Theta^{1136}_{E_gE_gT_{1u}T_{1u}} = 14.606, \Theta^{1144}_{E_gE_gT_{1u}T_{1u}} = 2.133, \Theta^{1155}_{E_gE_gT_{1u}T_{1u}} = 5.333, \Theta^{1166}_{E_gE_gT_{1u}T_{1u}} = 5.333, \Theta^{1222}_{E_gE_gT_{1u}T_{1u}} = -6.928, \Theta^{1225}_{E_gE_gT_{1u}T_{1u}} = -10.119, \Theta^{1233}_{E_gE_gT_{1u}T_{1u}} = 6.928, \Theta^{1236}_{E_gE_gT_{1u}T_{1u}} = 10.119, \Theta^{1255}_{E_gE_gT_{1u}T_{1u}} = -3.695, \Theta^{1266}_{E_gE_gT_{1u}T_{1u}} = 3.695, \Theta^{2211}_{E_gE_gT_{1u}T_{1u}} = 12.0, \Theta^{2214}_{E_gE_gT_{1u}T_{1u}} = 17.527, \Theta^{2222}_{E_gE_gT_{1u}T_{1u}} = 6.0, \Theta^{2225}_{E_gE_gT_{1u}T_{1u}} = 8.764, \Theta^{2233}_{E_gE_gT_{1u}T_{1u}} = 6.0, \Theta^{2236}_{E_gE_gT_{1u}T_{1u}} = 8.764, \Theta^{2244}_{E_gE_gT_{1u}T_{1u}} = 6.4, \Theta^{2255}_{E_gE_gT_{1u}T_{1u}} = 3.2, \Theta^{2266}_{E_gE_gT_{1u}T_{1u}} = 3.2$
143	$\Theta^{1111}_{A_{1g}A_{1g}T_{2g}T_{2g}} = 16.0, \Theta^{1122}_{A_{1g}A_{1g}T_{2g}T_{2g}} = 16.0, \Theta^{1133}_{A_{1g}A_{1g}T_{2g}T_{2g}} = 16.0$
144	$\Theta^{1122}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 16.0, \Theta^{1125}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 23.369, \Theta^{1155}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 8.533, \Theta^{2233}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 16.0, \Theta^{2236}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 23.369, \Theta^{2266}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 8.533, \Theta^{3311}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 16.0, \Theta^{3314}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 23.369, \Theta^{3344}_{T_{1g}T_{1g}T_{1u}T_{1u}} = 8.533$
145	$\Theta^{1122}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 8.533, \Theta^{1125}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 23.369, \Theta^{1155}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 16.0, \Theta^{2233}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 8.533, \Theta^{2236}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 23.369, \Theta^{2266}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 16.0, \Theta^{3311}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 8.533, \Theta^{3314}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 23.369, \Theta^{3344}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 16.0$
146	$\Theta^{1111}_{E_gE_gT_{1u}T_{1u}} = 12.0, \Theta^{1114}_{E_gE_gT_{1u}T_{1u}} = 17.527, \Theta^{1122}_{E_gE_gT_{1u}T_{1u}} = 6.0, \Theta^{1125}_{E_gE_gT_{1u}T_{1u}} = 8.764, \Theta^{1133}_{E_gE_gT_{1u}T_{1u}} = 6.0, \Theta^{1136}_{E_gE_gT_{1u}T_{1u}} = 8.764, \Theta^{1144}_{E_gE_gT_{1u}T_{1u}} = 6.4, \Theta^{1155}_{E_gE_gT_{1u}T_{1u}} = 3.2, \Theta^{1166}_{E_gE_gT_{1u}T_{1u}} = 3.2, \Theta^{1222}_{E_gE_gT_{1u}T_{1u}} = 6.928, \Theta^{1225}_{E_gE_gT_{1u}T_{1u}} = 10.119, \Theta^{1233}_{E_gE_gT_{1u}T_{1u}} = -6.928, \Theta^{1236}_{E_gE_gT_{1u}T_{1u}} = -10.119, \Theta^{1255}_{E_gE_gT_{1u}T_{1u}} = 3.695, \Theta^{1266}_{E_gE_gT_{1u}T_{1u}} = -3.695, \Theta^{2211}_{E_gE_gT_{1u}T_{1u}} = 4.0, \Theta^{2214}_{E_gE_gT_{1u}T_{1u}} = 5.842, \Theta^{2222}_{E_gE_gT_{1u}T_{1u}} = 10.0, \Theta^{2225}_{E_gE_gT_{1u}T_{1u}} = 14.606, \Theta^{2233}_{E_gE_gT_{1u}T_{1u}} = 10.0, \Theta^{2236}_{E_gE_gT_{1u}T_{1u}} = 14.606, \Theta^{2244}_{E_gE_gT_{1u}T_{1u}} = 2.133, \Theta^{2255}_{E_gE_gT_{1u}T_{1u}} = 5.333, \Theta^{2266}_{E_gE_gT_{1u}T_{1u}} = 5.333$

147	$\Theta^{1111}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 11.685, \Theta^{1114}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 41.6, \Theta^{1144}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 53.75, \Theta^{1444}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 30.151, \Theta^{2222}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 11.685, \Theta^{2225}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 41.6, \Theta^{2255}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 53.75, \Theta^{2555}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 30.151, \Theta^{3333}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 11.685, \Theta^{3336}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 41.6, \Theta^{3366}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 53.75, \Theta^{3666}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 30.151, \Theta^{4444}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 6.232, \Theta^{5555}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 6.232, \Theta^{6666}_{T_{1u}T_{1u}T_{1u}T_{1u}} = 6.232$
148	$\Theta^{1122}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 11.685, \Theta^{1125}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 24.533, \Theta^{1155}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 11.685, \Theta^{2233}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 11.685, \Theta^{2236}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 24.533, \Theta^{2266}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 11.685, \Theta^{3311}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 11.685, \Theta^{3314}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 24.533, \Theta^{3344}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 11.685$
149	$\Theta^{1223}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 16.0, \Theta^{1226}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 11.685, \Theta^{1235}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 11.685, \Theta^{1256}_{T_{2g}T_{2g}T_{1u}T_{1u}} = 8.533, \Theta^{1312}_{T_{2g}T_{2g}T_{1u}T_{1u}} = -16.0, \Theta^{1315}_{T_{2g}T_{2g}T_{1u}T_{1u}} = -11.685, \Theta^{1324}_{T_{2g}T_{2g}T_{1u}T_{1u}} = -11.685, \Theta^{1345}_{T_{2g}T_{2g}T_{1u}T_{1u}} = -8.533, \Theta^{2313}_{T_{2g}T_{2g}T_{1u}T_{1u}} = -16.0, \Theta^{2316}_{T_{2g}T_{2g}T_{1u}T_{1u}} = -11.685, \Theta^{2334}_{T_{2g}T_{2g}T_{1u}T_{1u}} = -11.685, \Theta^{2346}_{T_{2g}T_{2g}T_{1u}T_{1u}} = -8.533$
150	$\Theta^{1112}_{A_{1g}T_{2g}T_{2u}T_{2u}} = -16.0, \Theta^{1223}_{A_{1g}T_{2g}T_{2u}T_{2u}} = 16.0, \Theta^{1313}_{A_{1g}T_{2g}T_{2u}T_{2u}} = 16.0$
151	$\Theta^{1111}_{A_{1g}A_{1g}E_gE_g} = 24.0, \Theta^{1122}_{A_{1g}A_{1g}E_gE_g} = 24.0$
152	$\Theta^{1123}_{A_{1g}T_{2g}T_{2g}T_{2g}} = 48.0$
153	$\Theta^{1111}_{A_{1g}E_gE_gE_g} = 12.0, \Theta^{1122}_{A_{1g}E_gE_gE_g} = -36.0$